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Fig. 1

TITIE: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE

Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Express Mail No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000)

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REMARK S. aureus Thymidylate kinase coordinates r= 0.236579 free r= 0.308425 REMARK DATE:16-Jun-99 10:01:57 49.8 CRYST1 90.1 46.5 90.00 101.80 90.00 P 2 1 2 Z Occ B Y 15.565 30.611 7.591 1.00 45.66 MOTA 1 Ν GLY 2223 Α $\bar{2}$ 6.969 GLY 16.755 1.00 45.93 MOTA CA 31.162 Α 17.911 18.705 31.377 32.317 7.940 7.758 MOTA 3 С GLY 1.00 46.18 Α MOTA 4 0 GLY 1.00 48.32 Α 17.998 5 30.531 8.975 MOTA N SER 1.00 42.96 Α 3 19.072 9.970 1.00 39.00 MOTA 6 CA SER 30.610 Α 7 11.292 **MOTA** CB SER 18.627 29.966 1.00 40.17 Α 19.120 20.281 12.402 9.397 8 3 30.700 1.00 40.63 Α MOTA OG SER 3 9 С 29.874 1.00 36.56 Α MOTA SER 10 3 29.839 8.181 1.00 39.31 20.446 Α MOTA 0 SER 11 ALA 4 21.128 29.286 10.238 1.00 31.10 Α MOTA Ν 22.288 1.00 25.76 12 CA ALA 4 28.569 9.699 Α MOTA 29.356 1.00 29.23 13 CB 23.547 10.017 **MOTA** ALA 4 Α 14 C 4 22.454 27.088 10.136 1.00 21.31 ATOM ALA 1.00 18.84 MOTA 15 0 ALA 23.384 26.753 10.865 Α MOTA 16 PHE 5 5 5 21.574 26.211 9.653 1.00 17.80 Α N 9.982 MOTA 17 CA PHE 21.613 24.783 1.00 15.57 Α 1.00 15.42 18 20.202 24.333 10.411 Α MOTA CB PHE 5 22.891 19 20.106 10.864 1.00 9.82 Α MOTA CG PHE 5 11.241 20 1.00 7.80 Α MOTA CD1 PHE 21.231 22.181 5 18.874 22.243 10.880 1.00 12.23 Α 21 CD2 PHE MOTA MOTA 22 55555 21.134 20.852 11.625 1.00 10.94 Α CE1 PHE 18.773 23 **ATOM** CE2 PHE 20.911 11.266 1.00 12.85 Α 11.633 MOTA 24 CZPHE 19.907 20.217 1.00 9.60 Α MOTA 25 C PHE 22.100 23.956 8.782 1.00 15.42 Α 26 21.319 23.382 MOTA 0 PHE 23.652 7.880 1.00 15.73 Α 6 27 MOTA Ν ILE 23.587 8.776 1.00 14.77 Α 23.960 25.224 6 28 22.816 7.669 MOTA CA ILE 1.00 14.44 Α 29 6 7.094 1.00 14.35 MOTA CB ILE 23.507 Α 6 22.739 30 CG2 ILE 25.740 5.899 1.00 13.40 MOTA Α CG1 6 24.911 24.947 6.685 1.00 12.20 Α MOTA 31 ILE32 6 26.136 25.851 6.740 1.00 11.34 MOTA CD1 ILE Α 8.108 33 6 24.373 21.413 1.00 13.52 Α MOTA C ILE 34 35 6 7 24.948 9.177 MOTA ILE 21.245 1.00 11.51 0 Α 24.100 7.258 1.00 14.2920.421 MOTA N THR Α 7 24.440 7.532 1.00 16.52 Α MOTA 36 CA THR 19.020 37 7 23.198 18.154 7.544 1.00 18.14 Α MOTA CB THR 1.00 20.48 1.00 20.31 7 22.475 6.322 **ATOM** 38 OG1 THR 18.365 Α 18.494 8.753 MOTA 39 CG2 THR 7 22.314 Α 7 25.355 40 18.480 6.437 1.00 16.16 Α MOTA С THR 7 1.00 16.42 MOTA 41 0 25.217 18.846 5.274 Α THR ATOM 42 N PHE 8 26.278 17.598 6.795 1.00 16.88 Α 43 CA 8 27.193 5.799 1.00 17.17 ATOM PHE 17.053 Α 17.250 18.704 44 CB 8 28.647 6.259 1.00 16.14 ATOM PHE Α 6.285 7.206 5.387 7.238 8 MOTA 45 CG PHE 29.094 1.00 17.67 Α MOTA 46 CD1 PHE 8 28.549 19.600 1.00 17.53 Α 47 8 30.059 19.177 1.00 16.84 ATOM CD2 PHE Α 48 8 28.960 20.935 1.00 13.97 ATOM CE1 PHE Α 49 8 30.479 20.519 5.412 CE2 1.00 12.30 MOTA PHE Α 50 CZ8 29.924 21.393 6.336 1.00 14.49 Α MOTA PHE 5.550 15.579 8 26.914 1.00 17.25 51 С PHE Α ATOM 14.755 8 27.194 6.394 52 0 PHE 1.00 18.79 Α **ATOM**

Fig. 2

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
345678901234567890123456789012345678901234567890123456789012345678901234567890123456789
N GLU CA GLU CB GLU CB GLU CG GLU OE1 GLU OE2 GLU OE2 GLU C GLU C GLU OE3 GLU C GLU
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26.0694 3594 36.0654 26.0691 26.069
15.249 13.8749 14.249 13.7273 13.3659 14.3659 13.6268 11.3936
4.388 4.34835 4.329 5.6900 3.4329 5.6939 3.4322 2.9880 2.4822 2.9880 2.4823 2.4882 2.4883 2.4883 2.4884 1.5944 1.5944 1.6377 2.773.3928 1.7923 2.773.3928 1.7923 2.773.3928 1.7923 2.7733 2.7
1.00 17.51 1.00 17.55 1.00 17.76 1.00 20.61 1.00 23.30 1.00 22.58 1.00 26.41 1.00 18.24 1.00 16.08 1.00 19.97 1.00 20.35 1.00 20.35 1.00 20.37 1.00 20.79 1.00 21.56 1.00 18.77 1.00 21.56 1.00 18.77 1.00 21.58 1.00 21.56 1.00 19.74 1.00 33.39 1.00 35.99 1.00 39.53 1.00 34.50 1.00 17.26 1.00 18.42 1.00 17.26 1.00 17.26 1.00 18.42 1.00 17.26 1.00 18.42 1.00 17.26 1.00 18.42 1.00 17.78 1.00 16.87 1.00 15.78 1.00 16.79 1.00 15.93 1.00 22.08 1.00 23.73 1.00 20.26 1.00 17.48 1.00 17.42 1.00 15.45 1.00 15.45 1.00 20.99 1.00 20.95 1.00 20.95 1.00 20.95 1.00 20.95
A A A A A A A A A A A A A A A A A A A

Fig. 2A-1

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	0112345678901234567890112341111111111111111111111111111111111	C THR O THR N THR CA THR CB THR CG2 THR OG1 THR CG2 THR O THR CG2 VAL CG VAL CG3 VAL CG4 VAL CG5 VAL CG6 VAL CG6 VAL CG7 VAL CG8 ILE CG7 ILE CG7 ILE CG7 ILE CG8 ASN CG8 ASN CG9 ASN CG9 ASN CC9 ASN CC9 CC9 GLU CC9 GLU CC9	17 18 18 18 18 19 19 19 19 20 20 20 21 21 21 21 22 22 22 22 22 22 22 22 22	36.711 37.215 38.319 40.0212 38.319 40.0715 38.17529 36.122 38.1752 36.123 36.123 36.123 36.123 37.733 31.593 31.5	15.222 16.021 15.221 16.176 15.614 16.731 17.464 16.731 18.539 18.539 17.218 18.320 17.218 18.321 19.546 19.546 19.024 19.024 19.024 19.025 19.025 19.026 19.026 19.026 19.026 19.026 19.027 19	8.4215 9.3406 1.3406	1.00 21.60 1.00 19.85 1.00 19.88 1.00 19.26 1.00 21.08 1.00 20.76 1.00 17.35 1.00 15.07 1.00 15.71 1.00 15.71 1.00 15.71 1.00 21.42 1.00 21.42 1.00 21.42 1.00 25.65 1.00 25.65 1.00 25.65 1.00 25.65 1.00 25.88 1.00 25.88 1.00 25.88 1.00 25.88 1.00 25.88 1.00 25.88 1.00 25.88 1.00 25.88 1.00 27.70 1.00 39.00 1.00 37.51 1.00 27.50 1.00 2	7. 7. 7. 7. 7. 7.
ATOM ATOM ATOM ATOM ATOM	151 152 153 154 155	N VAL CA VAL CB VAL CG1 VAL CG2 VAL	23 23 23 23 23	36.672 35.745 34.451 33.282 34.679	22.992 24.042 23.455 24.425 23.165	6.823 6.436 5.803 5.968 4.323	1.00 21.05 1.00 19.39 1.00 19.91 1.00 16.41 1.00 16.29	7 7 7 7 7 7 7 7 7 7 7

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
168 169 171 172 173 174 175 177 178 181 182 183 184 185 189 191 193 194 195 197 198 199 201 202 203 203 203 203 203 203 203 203 203
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2444555555555666666666777777778888889999999999
34.973 36.757 37.229 38.324 39.833 39.833 40.738 39.833 40.738 39.906 39.788 39.2967 37.886 39.2967 37.886 39.2967 37.896 39.2967 39.2
25.614 25.699 26.886 26.209 25.241 24.810 25.621 24.810 25.621 24.810 27.221 28.300 27.310 28.371
16.501 10.556 10.719 10.734 11.166 11.141 12.374 13.656 12.396 13.625 14.417 10.349 10.731 9.225 8.3868 5.852 4.864 3.475 2.431 1.200 8.594 8.609 10.415 11.399 12.735 13.755 13.754 11.663 10.357 10.230 9.454 11.751 11.053 11.091 9.8896 8.2649 11.788
1.00 13.33 1.00 14.44 1.00 13.95 1.00 15.76 1.00 20.04 1.00 21.45 1.00 25.49 1.00 27.02 1.00 27.27 1.00 28.81 1.00 29.55 1.00 21.20 1.00 23.69 1.00 23.69 1.00 25.23 1.00 26.42 1.00 30.95 1.00 32.99 1.00 33.53 1.00 26.52 1.00 27.39 1.00 24.86 1.00 26.52 1.00 23.07 1.00 24.86 1.00 19.14 1.00 19.04 1.00 19.04 1.00 19.14 1.00 19.04 1.00 19.75 1.00 20.53 1.00 20.53 1.00 20.53 1.00 20.53 1.00 20.53 1.00 20.53 1.00 20.53 1.00 20.76 1.00 23.32 1.00 22.92 1.00 23.32 1.00 22.92 1.00 23.32 1.00 22.92 1.00 23.32 1.00 22.70 1.00 24.04 1.00 22.62 1.00 23.35 1.00 20.31 1.00 22.92 1.00 23.32 1.00 22.70 1.00 24.04 1.00 22.62 1.00 23.55 1.00 20.31 1.00 22.70 1.00 24.04 1.00 22.62 1.00 23.55 1.00 20.31 1.00 22.70 1.00 24.04 1.00 22.62 1.00 23.32 1.00 22.70 1.00 24.04 1.00 25.21 1.00 24.91 1.00 26.90 1.00 28.76 1.00 34.03 1.00 32.19 1.00 24.87
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA

Fig. 2A-3

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MOTA	224	CA	TYR	31	31.172	33.259	11.966		22.02	Α
ATOM	225	CB	TYR	31	30.843	32.192	10.917		20.30	A
ATOM	226	CG	TYR	31	30.526	32.735	9.555		16.72	A
MOTA	227 228	CD1 CE1	TYR	31 31	31.502	32.773	8.571		18.10 17.46	A A
ATOM ATOM	228	CD2	TYR TYR	31	31.236 29.259	33.262 33.202	7.305 9.245		15.65	A
ATOM	230	CE2	TYR	31	28.974	33.700	7.973		17.00	A
ATOM	231	CZ	TYR	31	29.974	33.724	7.006		17.27	A
ATOM	232	ОH	TYR	31	29.735	34.202	5.736		17.42	A
ATOM	233	С	TYR	31	31.086	32.598	13.331		20.05	Α
ATOM	234	0	TYR	31	32.075	32.092	13.850		20.06	Α
MOTA	235	N	ASP	32	29.892	32.622	13.908		19.70	A
ATOM	236	CA	ASP	32	29.636	31.990	15.190		20.95	A
ATOM ATOM	237 238	CB CG	ASP ASP	32 32	28.510 28.440	32.735 32.413	15.906 17.373		22.89 24.21	A A
ATOM	239	OD1	ASP	32	27.454	32.838	18.020		25.96	Ā
ATOM	240		ASP	32	29.363	31.739	17.872		24.55	A
ATOM	241	С	ASP	32	29.181	30.597	14.751		20.33	Α
ATOM	242	0	ASP	32	27.988	30.300	14.671		19.92	Α
ATOM	243	N	VAL	33	30.148	29.753	14.424		18.61	A
ATOM	244	CA	VAL	33	29.838	28.425	13.935		16.48	A
ATOM ATOM	245 246	CB CG1	VAL VAL	33 33	30.649 32.097	28.127 27.831	12.640 12.972		15.36 13.65	A A
ATOM	247	CG2		33	30.022	26.967	11.892		16.60	Ā
ATOM	248	C	VAL	33	30.077	27.337	14.968		16.76	A
MOTA	249	Ö	VAL	33	30.983	27.426	15.800		17.16	A
ATOM	250	N	ILE	34	29.241	26.306	14.910		15.58	Α
ATOM	251	CA	ILE	34	29.349	25.184	15.827		13.80	A
ATOM	252	CB	ILE	34	28.030	25.020 23.729	16.669		12.79 11.57	A
ATOM ATOM	253 254	CG2 CG1	ILE ILE	34 34	28.049 27.919	26.145	17.474 17.680		11.37	A A
ATOM	255	CD1	ILE	34	29.120	26.219	18.560		10.18	A
ATOM	256	C	ILE	34	29.608	23.929	14.992		13.84	A
ATOM	257	0	ILE	34	29.024	23.758	13.921		12.61	Α
MOTA	258	N	MET	35	30.506	23.080	15.496		15.72	A
ATOM	259	CA	MET	35	30.888	21.815	14.873		16.23	A
ATOM ATOM	260 261	CB CG	MET MET	35 35	32.418 32.988	21.717 21.367	14.811 13.441		13.95 15.83	A A
ATOM	262	SD	MET	35	34.670	20.692	13.593		12.02	A
ATOM	263	ČE	MET	35	34.279	18.976	13.591		15.12	A
ATOM	264	С	MET	35	30.342	20.672	15.746		16.39	Α
MOTA	265	0	MET	35	30.740	20.533	16.903	1.00		A
ATOM	266	N	THR	36	29.451	19.849	15.189	1.00 1		A
ATOM ATOM	267 268	CA CB	THR THR	36 36	28.859 27.598	18.747 19.244	15.952 16.748		18.63 20.00	A A
ATOM	269	OG1	THR	36	27.292	18.337	17.817		18.36	A
ATOM	270	CG2	THR	36	26.395	19.337	15.833		18.79	A
ATOM	271	C	THR	36	28.453	17.518	15.117		18.55	A
ATOM	272	0	THR	36	28.268	17.592	13.908		16.66	Α
MOTA	273	N	ARG	37	28.336	16.382	15.801		20.67	A
ATOM	274	CA	ARG	37	27.913	15.108	15.224		20.65	A
ATOM ATOM	275 276	CB CG	ARG ARG	37 37	29.115 30.170	14.269 14.129	14.796 15.855	1.00 2 $1.00 2$	21.76	A A
ATOM	277	CD	ARG	37	31.559	14.129	15.239		35.37	A
ATOM	278	NE	ARG	37	32.614	14.108	16.256	1.00		A
ATOM	279	CZ	ARG	37	33.904	14.297	15.998	1.00	42.90	Α
ATOM	280		ARG	37	34.780	14.315	16.995	1.00	44.86	Α

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
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NH2 NH2 ON CBGCCOCCOONCCOONCCOONCCCCCOONCCCOONCCCOONCCCCCOONCCCCCC
GLU GLU PRO PRO PRO PRO PRO PRO GLY GLY GLY GLY GLY GLY CLY CLY VAL VAL VAL
37 37 38 38 38 38 38 38 39 39 39 40 40 41 41 41 42 42 42 42 42 43 43 44 44 44 44 44 44 44 44 44 44 44
34.321 27.186 27.746 25.937 23.692 22.092 22.1855 25.485 25.485 25.485 25.485 25.485 26.285 27.642 27.7642 27.642 27.7662 27.7642 27.7662 27.7
14.468 14.428 14.279 14.038 13.243 12.317 11.387 13.433 12.066 11.298 11.760 10.461 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 10.466 11.533 11.792 15.4829 15.4829 15.493 11.7991 11.7991 11.7991 11.7991 11.7991 11.666 11.7991
14.745 16.378 17.466 16.147 17.182 16.751 11.761 13.9745 14.761 13.9745 14.761 13.9745 17.6876 19.0055
1.00 45.05 1.00 19.50 1.00 16.50 1.00 20.18 1.00 22.89 1.00 21.85 1.00 21.08 1.00 24.03 1.00 24.77 1.00 24.13 1.00 26.42 1.00 26.55 1.00 27.84 1.00 26.55 1.00 27.84 1.00 29.42 1.00 29.69 1.00 29.69 1.00 29.69 1.00 27.71 1.00 28.44 1.00 28.44 1.00 28.44 1.00 27.66 1.00 27.35 1.00 27.35 1.00 27.35 1.00 27.35 1.00 27.55 1.00 27.55 1.00 27.55 1.00 27.55 1.00 26.03 1.00 27.70 1.00 30.35 1.00 27.70 1.00 30.35 1.00 35.84 1.00 38.67
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тпом	220	0.11	OT 11	1.0	07 100	11 165	22 000	1 00 40 57	70
ATOM ATOM	338 339	OE1 OE2	GLU GLU	46 46	27.188 28.358	11.165 11.749	23.090 24.855	1.00 40.57 1.00 39.83	A A
ATOM	340	C	GLU	46	24.038	7.882	25.336	1.00 28.82	A
ATOM	341	0	GLU	46	24.499	6.783	25.016	1.00 29.81	Α
ATOM	342	N	GLU	47	23.079	8.026	26.251	1.00 29.16	A
MOTA	343	CA	GLU	47	22.507	6.899	26.981	1.00 28.33	A
ATOM ATOM	344 345	CB CG	GLU GLU	47 47	21.505 21.919	7.370 8.575	28.032 28.821	1.00 31.03 1.00 35.69	A A
ATOM	346	CD	GLU	47	22.509	8.193	30.155	1.00 33.03	A
ATOM	347	OE1	GLU	47	21.965	7.267	30.806	1.00 38.20	A
ATOM	348	OE2	GLU	47	23.519	8.821	30.544	1.00 41.18	Α
ATOM	349	C	GLU	47	21.772	5.982	26.041	1.00 28.66	A
ATOM	350	0	GLU	47	21.953	4.772	26.070	1.00 28.63	A
ATOM ATOM	351 352	N CA	ILE ILE	48 48	20.902 20.132	6.570 5.801	25.230 24.273	1.00 28.67 1.00 29.14	A A
ATOM	353	CB	ILE	48	19.149	6.705	23.496	1.00 27.61	A
ATOM	354	CG2	ILE	48	18.185	5.857	22.700	1.00 26.69	Α
ATOM	355	CG1	ILE	48	18.388	7.613	24.470	1.00 26.60	A
MOTA	356	CD1	ILE	48	17.490	8.628	23.793 23.304	1.00 25.71 1.00 29.77	A
ATOM ATOM	357 358	C	ILE ILE	48 48	21.115 20.959	5.162 4.006	23.304	1.00 29.77	A A
ATOM	359	N	ARG	49	22.135	5.927	22.934	1.00 32.23	A
ATOM	360	CA	ARG	49	23.160	5.461	22.014	1.00 36.58	A
ATOM	361	CB	ARG	49	24.187	6.577	21.777	1.00 38.28	A
ATOM ATOM	362 363	CG CD	ARG ARG	49 49	24.753 23.682	6.621 7.033	20.375 19.373	1.00 40.84 1.00 44.51	A A
ATOM	364	NE	ARG	49	24.221	7.033	18.240	1.00 47.33	A
ATOM	365	CZ	ARG	49	25.323	7.452	17.570	1.00 47.80	A
MOTA	366	NH1	ARG	49	26.018	6.372	17.914	1.00 47.10	A
ATOM	367	NH2		49	25.725	8.194	16.548	1.00 46.92	A
ATOM ATOM	368 369	C 0	ARG ARG	49 49	23.862 24.019	4.227 3.208	22.585 21.909	1.00 38.44 1.00 40.42	A A
ATOM	370	N	LYS	50	24.278	4.328	23.841	1.00 38.03	A
ATOM	371	CA	LYS	50	24.975	3.248	24.525	1.00 36.83	Α
ATOM	372	CB	LYS	50	25.279	3.684	25.952	1.00 37.35	A
ATOM	373 374	CG	LYS	50	25.964 27.429	2.626 2.960	26.796 27.030	1.00 40.72 1.00 41.37	A A
ATOM ATOM	375	CD CE	LYS LYS	50 50	27.429	4.392	27.030	1.00 41.37	A
ATOM	376	ΝZ	LYS	50	29.032	4.798	27.561	1.00 47.85	A
ATOM	377	С	LYS	50	24.213	1.919	24.551	1.00 36.69	Α
ATOM	378	0	LYS	50	24.817	0.854	24.671	1.00 35.81	A
ATOM ATOM	379 380	N CA	ILE ILE	51 51	22.890 22.062	1.982 0.782	24.439 24.474	1.00 35.96 1.00 35.56	A A
ATOM	381	CB	ILE	51	20.577	1.141	24.612	1.00 34.05	A
ATOM	382	CG2	ILĒ	51	19.714	-0.058	24.261	1.00 31.47	Α
ATOM	383	CG1	ILE	51	20.306	1.607	26.043	1.00 33.91	A
ATOM	384	CD1	ILE	51	18.863	1.928	26.333	1.00 36.27	A
ATOM ATOM	385 386	C 0	ILE ILE	51 51	22.235 22.362	-0.110 -1.324	23.258 23.388	1.00 37.00 1.00 36.83	A A
ATOM	387	Ň	VAL	52	22.237	0.489	22.076	1.00 38.92	A
ATOM	388	CA	VAL	52	22.391	-0.282	20.858	1.00 41.12	Α
ATOM	389	CB	VAL	52	22.120	0.601	19.604	1.00 40.76	A
ATOM ATOM	390 391	CG1 CG2	VAL VAL	52 52	23.142 22.133	1.688 -0.244	19.508 18.341	1.00 42.48 1.00 41.09	A A
ATOM	392	C	VAL	52	23.798	-0.873	20.805	1.00 42.70	A
ATOM	393	Ō	VAL	52	23.992	-2.003	20.348	1.00 43.15	A
ATOM	394	N	LEU	53	24.766	-0.120	21.319	1.00 44.83	Α

Fig. 2A-6

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	395 396 397 398 399 400 401 402 403 404 405 406 407 408 409	CB CG CD CA CB CC CD CC	LEU LEU LEU LEU LEU LEU GLU GLU GLU GLU GLU GLU GLU	53 53 53 53 53 54 54 54 54 54 54	26.171 27.054 27.020 27.969 27.393 26.536 27.392 25.908 26.215 26.523 27.503 28.865 28.918 29.888 25.129	-0.528 0.640 1.876 2.933 1.480 -1.773 -2.553 -1.966 -3.135 -2.696 -1.501 -1.856 -2.722 -1.256 -4.219	21.313 21.762 20.855 21.381 19.436 22.115 21.689 23.272 24.099 25.546 25.668 26.291 27.194 25.878 24.075 25.068	1.00 47.39 1.00 45.93 1.00 44.42 1.00 43.88 1.00 44.16 1.00 49.72 1.00 50.88 1.00 52.50 1.00 55.23 1.00 57.10 1.00 60.18 1.00 61.65 1.00 62.65 1.00 62.65 1.00 54.90 1.00 55.38	A A A A A A A A A A A A A A A A A A A
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	410 411 412 413 414 415 416 417 418 420 421 422 423 424 425 426 427 428	N CA CB CG N CA CB CC	GLU GLY GLY GLY ASN ASN ASN ASN ASN ASP ASP ASP	54 555 555 556 556 557 577 57	24.898 24.465 23.440 23.817 23.789 24.157 24.625 25.190 24.455 24.993 23.221 23.739 23.919 22.826 21.994 21.827 21.377 22.745	-4.905 -4.359 -5.380 -5.965 -5.235 -7.257 -7.847 -9.264 -10.052 -11.018 -9.661 -7.856 -7.016 -8.813 -8.847 -10.282 -11.325 -11.162 -12.310	22.928 22.727 21.372 20.378 21.308 20.248 21.301 21.848 21.588 18.781 17.898 18.657 17.457 16.941 18.036 19.115 17.813	1.00 55.29 1.00 56.52 1.00 57.57 1.00 58.88 1.00 57.61 1.00 58.29 1.00 59.27 1.00 61.14 1.00 60.14 1.00 56.28 1.00 57.68 1.00 57.68 1.00 53.31 1.00 49.64 1.00 60.39 1.00 62.29 1.00 62.30	A A A A A A A A A A A A A A A A A A A
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	429 430 431 432 433 434 435 436 437 438 441 442 443 444 445 446	C A I CB I CC I CC I CC I CC I CC I CC I	ASP ASP MET MET MET MET MET MET ASP ASP ASP ASP	557 555 555 555 555 555 555 555 555 555	20.628 19.614 20.614 19.386 19.721 18.538 19.065 20.309 18.589 19.157 17.273 16.418 14.951 14.004 13.480 13.780 16.843 17.139	-8.237 -8.237 -8.921 -6.939 -6.213 -4.856 -4.129 -2.559 -3.111 -6.008 -5.727 -6.157 -5.960 -5.899 -5.615 -6.583 -4.428 -4.637 -3.679	17.715 17.648 17.999 18.266 18.873 19.490 20.141 21.333 16.987 15.934 17.085 15.928 16.370 15.220 14.629 14.629 14.629 16.004	1.00 44.53 1.00 44.53 1.00 43.89 1.00 37.61 1.00 27.21 1.00 21.68 1.00 13.77 1.00 15.00 1.00 28.14 1.00 28.52 1.00 23.91 1.00 22.60 1.00 23.15 1.00 24.20 1.00 24.88 1.00 25.85 1.00 21.41 1.00 19.52	A A A A A A A A A A A A A A A A
ATOM ATOM ATOM ATOM ATOM	447 448 449 450 451	N CA CB	ILE ILE ILE ILE	60 60 60 60	16.886 17.296 17.653 18.920 16.505	-4.583 -3.365 -3.638 -4.455 -4.347	13.963 13.279 11.808 11.733 11.112	1.00 22.14 1.00 21.20 1.00 18.94 1.00 18.95 1.00 17.72	A A A A

Fig. 2A-7

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ATOM	452	CD1	ILE	60	16.510	-4.136	9.614	1.00 17.04	А
ATOM	453	С	ILE	60	16.277	-2.226	13.354	1.00 21.86	Α
MOTA	454	0	ILE	60	16.653	-1.054	13.317	1.00 22.47	A
MOTA	455	N	ARG	61	14.993	-2.554	13.453	1.00 19.83	A
ATOM	456	CA	ARG	61	13.975	-1.519	13.566	1.00 19.98	A
ATOM	457	CB	ARG	61	12.596	-2.126	13.394	1.00 20.07	A
ATOM	458	CG	ARG	61	12.292	-2.512	11.979	1.00 21.25	A
ATOM ATOM	459 460	CD	ARG	61	10.814	-2.675 -2.820	11.799 10.394	1.00 23.50 1.00 25.00	A
ATOM	460	NE CZ	ARG ARG	61 61	10.446 9.313	-2.820 -2.356	9.878	1.00 25.00	A A
ATOM	462	NH1	ARG	61	9.049	-2.530	8.593	1.00 27.02	A
ATOM	463	NH2	ARG	61	8.444	-1.709	10.650	1.00 31.61	A
ATOM	464	C	ARG	61	14.061	-0.875	14.944	1.00 19.84	A
ATOM	465	0	ARG	61	13.664	0.273	15.145	1.00 20.49	Α
ATOM	466	N	THR	62	14.587	-1.640	15.889	1.00 21.09	Α
MOTA	467	CA	THR	62	14.731	-1.208	17.269	1.00 19.87	A
ATOM	468	CB	THR	62	14.911	-2.442	18.194	1.00 20.87	A
ATOM	469	OG1	THR	62	13.694	-3.198	18.208	1.00 21.98	A
ATOM	470 471	CG2	THR	62 62	15.252	-2.027	19.618 17.425	1.00 19.80 1.00 19.52	A A
ATOM ATOM	471	C 0	THR THR	62 62	15.913 15.811	-0.263 0.771	18.094	1.00 19.32	A
ATOM	473	N	GLU	63	17.037	-0.604	16.804	1.00 10.25	A
ATOM	474	CA	GLU	63	18.220	0.250	16.903	1.00 18.99	A
ATOM	475	CB	GLU	63	19.471	-0.529	16.509	1.00 19.03	A
ATOM	476	CG	GLU	63	19.288	-1.491	15.381	1.00 21.37	Α
MOTA	477	CD	GLU	63	20.619	-2.034	14.930	1.00 25.03	Α
ATOM	478	OE1	GLU	63	21.082	-1.623	13.840	1.00 26.31	A
ATOM	479	OE2	GLU	63	21.212	-2.856	15.664	1.00 25.70	A
ATOM	480	C	GLU	63	18.088	1.509	16.050	1.00 17.94	A
ATOM ATOM	481 482	O N	GLU ALA	63 64	18.832 17.138	2.467 1.491	16.211 15.132	1.00 21.25 1.00 15.64	A A
ATOM	483	CA	ALA	64	16.899	2.641	14.297	1.00 15.57	A
ATOM	484	CB	ALA	64	16.143	2.223	13.003	1.00 13.61	A
ATOM	485	Č	ALA	64	16.037	3.575	15.172	1.00 15.81	A
ATOM	486	0	ALA	64	16.356	4.752	15.363	1.00 16.61	Α
ATOM	487	N	MET	65	14.974	3.018	15.743	1.00 13.79	A
ATOM	488	CA	MET	65	14.087	3.794	16.604	1.00 13.69	Α
ATOM	489	CB	MET	65	13.039	2.874	17.251	1.00 12.94	A
ATOM	490	CG	MET	65	11.582	3.210	16.978	1.00 11.73	A
ATOM ATOM	491 492	SD CE	MET MET	65 65	10.527 9.097	1.815 2.396	17.282 16.652	1.00 6.30 1.00 5.95	A A
ATOM	493	CE	MET	65	14.926	4.462	17.699	1.00 12.98	A
ATOM	494	Ö	MET	65	14.797	5.653	17.945	1.00 13.88	A
ATOM	495	Ň	LEU	66	15.781	3.678	18.357	1.00 13.83	A
ATOM	496	CA	LEU	66	16.629	4.188	19.433	1.00 13.28	Α
MOTA	497	CB	LEU	66	17.479	3.066	20.058	1.00 13.35	Α
ATOM	498	CG	LEU	66	16.816	2.125	21.081	1.00 15.56	A
ATOM	499	CD1		66	17.852	1.159	21.623	1.00 13.13	A
ATOM	500	CD2	LEU	66	16.210	2.910	22.238	1.00 14.87	A
ATOM ATOM	501 502	C	LEU	66 66	17.558 17.884	5.290 6.191	18.948 19.711	1.00 13.84 1.00 14.62	A A
ATOM	503	O N	LEU PHE	67	17.004	5.197	17.694	1.00 14.82	A
ATOM	504	CA	PHE	67	18.898	6.196	17.109	1.00 15.86	Ä
ATOM	505	CB	PHE	67	19.591	5.612	15.865	1.00 17.75	A
MOTA	506	CG	PHE	67	21.020	5.206	16.103	1.00 20.57	Α
MOTA	507		PHE	67	22.060	6.051	15.749	1.00 25.92	Α
MOTA	508	CD2	PHE	67	21.327	3.989	16.691	1.00 22.84	A

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ATOM	509	CE1	PHE	67	23.382	5.691	15.974	1.00 26.79	Α
ATOM	510	CE2	PHE	67	22.645	3.624	16.921	1.00 23.85	A
MOTA	511	CZ	PHE	67	23.674	4.475	16.563	1.00 23.88	Α
MOTA	512	С	PHE	67	18.092	7.441	16.742	1.00 14.03	Α
ATOM	513	0	PHE	67	18.580	8.570	16.807	1.00 12.55	Α
ATOM	514	N	ALA	68	16.843	7.212	16.364	1.00 13.48	A
ATOM	515	CA	ALA	68	15.953	8.298	16.022	1.00 14.76	A
MOTA	516	CB	ALA	68	14.606	7.734	15.543	1.00 16.19	Α
MOTA	517	C	ALA	68	15.742	9.196	17.249	1.00 16.89	Α
MOTA	518	0	ALA	68	15.695	10.427	17.121	1.00 16.90	Α
ATOM	519	N	ALA	69	15.633	8.556	18.422	1.00 17.12	A
ATOM	520	CA	ALA	69	15.410	9.209	19.715	1.00 14.85	A
ATOM	521	CB	ALA	69	14.931	8.187	20.734	1.00 13.25	Α
MOTA	522	C	ALA	69	16.668	9.888	20.216	1.00 16.30	Α
ATOM	523	0	ALA	69	16.610	10.831	21.000	1.00 14.16	A
ATOM	524	N	SER	70	17.811	9.374	19.779	1.00 17.73	A
ATOM	525	CA	SER	70	19.103	9.943	20.123	1.00 19.15	A
ATOM	526	CB	SER	70	20.195	8.894	19.867	1.00 17.01	A
ATOM	527	OG	SER	70	21.462	9.336	20.308	1.00 15.22	A
ATOM	528	C	SER	70	19.284	11.179	19.199 19.569	1.00 22.47 1.00 22.68	A
ATOM ATOM	529 530	O N	SER	70 71	19.919 18.700	12.180 11.102	18.001	1.00 22.00	A A
ATOM	531	N CA	ARG ARG	71	18.763	12.187	17.022	1.00 23.10	A
ATOM	532	CB	ARG	71	18.330	11.688	15.642	1.00 24.02	A
ATOM	533	CG	ARG	71	18.342	12.757	14.554	1.00 24.85	A
ATOM	534	CD	ARG	71	17.961	12.183	13.187	1.00 27.81	A
ATOM	535	NE	ARG	71	18.976	11.257	12.684	1.00 33.70	A
ATOM	536	CZ	ARG	71	18.776	9.957	12.474	1.00 36.24	A
ATOM	537	NH1	ARG	71	19.761	9.198	12.019	1.00 39.64	A
ATOM	538	NH2		71	17.591	9.413	12.713	1.00 36.44	Α
ATOM	539	С	ARG	71	17.848	13.320	17.447	1.00 24.53	Α
ATOM	540	0	ARG	71	17.976	14.444	16.972	1.00 26.57	Α
ATOM	541	N	ARG	72	16.916	13.014	18.336	1.00 26.02	Α
MOTA	542	CA	ARG	72	15.978	14.001	18.849	1.00 26.19	Α
ATOM	543	CB	ARG	72	14.686	13.301	19.269	1.00 27.68	A
ATOM	544	CG	ARG	72	13.643	14.229	19.823	1.00 30.87	A
ATOM	545	CD	ARG	72	12.452	14.321	18.897	1.00 32.04	A
ATOM	546	NE	ARG	72	11.528	15.370	19.321	1.00 32.80	A
ATOM ATOM	547	CZ	ARG ARG	72 72	11.423	16.554	18.728	1.00 34.02 1.00 30.93	A A
ATOM	548 549	NH1	ARG	72	10.554 12.188	17.441 16.849	19.185 17.678	1.00 30.93	A
ATOM	550		ARG	72	16.569	14.778	20.041	1.00 32.07	A
ATOM	551	ŏ	ARG	72	16.353	15.987	20.173	1.00 25.92	A
ATOM	552	Ň	GLU	73	17.318	14.089	20.901	1.00 23.88	A
ATOM	553	CA	GLU	.3 73	17.917	14.737	22.069	1.00 23.70	A
ATOM	554	CB	GLU	73	18.510	13.706	23.042	1.00 24.81	Α
ATOM	555	CG	GLU	73	17.470	12.934	23.861	1.00 27.04	A
ATOM	556	CD	GLU	73	16.527	13.841	24.631	1.00 27.69	Α
MOTA	557	OE1	GLU	73	15.377	14.044	24.180	1.00 26.28	Α
ATOM	558	OE2	GLU	73	16.943	14.349	25.694	1.00 32.51	Α
MOTA	559	С	GLU	73	19.004	15.682	21.620	1.00 21.89	A
MOTA	560	0	GLU	73	19.059	16.826	22.062	1.00 22.04	A
ATOM	561	N	HIS	74	19.872	15.189	20.744	1.00 20.57	A
ATOM	562	CA	HIS	74	20.972	15.979	20.197	1.00 19.43	A
ATOM	563	CB	HIS	74	21.698	15.169	19.104	1.00 19.74	A
ATOM	564	CG	HIS	74	22.772	15.927	18.381	1.00 18.47	A
MOTA	565	CDZ	HIS	74	24.069	16.156	18.689	1.00 17.84	A

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
6789012345678900123456789001234567890012345678900123456789001234567890012345678900123456789001234567890012345678900123456789001234567890012345678900123456789001234567890012345678900123456789000000000000000000000000000000000000
ND1 HIS CE1 HIS NE2 HIS C HIS
744445555555666667777777777777777777777
22.561 23.689 24.615 20.403 19.556 17.520 16.787 17.606 17.8017 17.408 17.3098 17.3098 17.3098 17.3098 17.3098 17.3098 17.315 18.647 17.510 21.315 21.315 22.988 22
16.519 17.070 17.070 17.070 17.0870 17.0870 17.0870 17.18.3429 17.18.4571 18.17.18.4571 18.17.19.18.6425 18.17.19.18.6425 18.22719.8447 18.22719.8447 18.22719.8447 18.22719.8447 18.32719.8447 18.32719.8447 18.32719.8447 19.328.6424 19.328.755 19.328
17.151 16.7394 17.6599 17.6599 18.92937 18.92937 18.92937 18.92937 18.9293 17.3795 18.9293 17.3795 18.9293 17.3795 18.9293 17.3795 18.9293 17.9293 18.9293 18.9293 18.9293 18.9293 18.9293 18.9393 17.9393 17.
1.00 15.64 1.00 14.64 1.00 18.09 1.00 17.65 1.00 17.62 1.00 16.80 1.00 17.58 1.00 16.00 1.00 16.84 1.00 17.06 1.00 14.46 1.00 19.92 1.00 19.25 1.00 21.23 1.00 23.42 1.00 23.42 1.00 24.71 1.00 24.71 1.00 24.71 1.00 24.71 1.00 24.22 1.00 25.02 1.00 24.22 1.00 25.02 1.00 24.22 1.00 25.02 1.00 24.22 1.00 25.02 1.00 24.28 1.00 24.28 1.00 27.57 1.00 26.45 1.00 27.57 1.00 28.49 1.00 19.94 1.00 16.59 1.00 19.94 1.00 16.55 1.00 16.63 1.00 19.94 1.00 16.55 1.00 16.63 1.00 17.68
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA

Fig. 2A-10

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ATOM	623	С	PRO	81	20.064	26.911	20.296	1.00 21.52	А
ATOM	624	0	PRO	81	19.884	28.096	20.032	1.00 24.42	A
ATOM	625		ALA	82	21.147	26.246	19.910	1.00 20.79	A
ATOM	626	CA	ALA	82	22.212	26.908	19.156	1.00 21.00	A
ATOM	627		ALA	82	23.231	25.883	18.682	1.00 19.36	A
MOTA	628 629	С	ALA ALA	82 82	21.681 22.167	27.709 28.808	17.966 17.685	1.00 20.35 1.00 21.95	A A
ATOM ATOM	630	N	LEU	83	20.684	27.163	17.277	1.00 19.97	Α
ATOM	631	CB	LEU	83	20.095	27.834	16.130	1.00 20.55	A
ATOM	632		LEU	83	19.140	26.887	15.386	1.00 18.99	A
ATOM	633		LEU	83	19.716	25.588	14.779	1.00 18.41	A
ATOM	634		LEU	83	18.705	24.977	13.822	1.00 15.72	A
ATOM	635		LEU	83	21.011	25.871	14.039	1.00 16.05	A
ATOM	636		LEU	83	19.349	29.086	16.588	1.00 23.59	A
ATOM	637	0	LEU	83	19.175	30.028	15.814	1.00 23.10	A
ATOM	638		LYS	84	18.921	29.094	17.850	1.00 25.75	A
ATOM	639	CA	LYS	84	18.192	30.232	18.416	1.00 27.61	A
ATOM	640		LYS	84	17.167	29.736	19.435	1.00 28.01	A
ATOM	641	CG	LYS	84	15.981	29.070	18.795 19.815	1.00 29.06 1.00 31.01	A A
ATOM ATOM	642 643	CE	LYS LYS	84 84	15.231 13.946	28.263 27.717	19.237	1.00 33.77	A
ATOM ATOM	644 645	С	LYS LYS	84 84	13.330	26.759 31.280	20.197	1.00 36.32	A A
ATOM	646	N	LYS	84	18.646	32.367	19.419	1.00 26.91	A
ATOM	647		GLU	85	20.373	30.928	19.235	1.00 28.01	A
ATOM	648		GLU	85	21.367	31.843	19.785	1.00 27.28	A
ATOM	649		GLU	85	22.469	31.075	20.523	1.00 29.14	A
ATOM	650		GLU	85	21.952	29.927	21.370	1.00 36.53	A
ATOM	651		GLU	85	23.062	29.140	22.070	1.00 42.07	A
ATOM	652		GLU	85	22.981	28.955	23.305	1.00 44.49	A
ATOM	653		GLU	85	24.018	28.702	21.391	1.00 44.75	A
ATOM	654	С	GLU	85	21.948	32.540	18.554	1.00 26.23	A
ATOM	655		GLU	85	22.845	33.378	18.661	1.00 26.25	A
ATOM ATOM	656 657	N	GLY GLY	86 86	21.410 21.828	32.167 32.717	17.389 16.111	1.00 26.07 1.00 26.47	A A
ATOM	658	С	GLY	86 86	23.140 23.925	32.717 32.155 32.897	15.589	1.00 26.47 1.00 26.86 1.00 29.40	A A
ATOM ATOM	659 660	N	GLY LYS	87	23.383	30.861	15.798	1.00 24.80	Α
ATOM ATOM	661 662	CB	LYS LYS	87 87	24.630 25.139	30.231 29.249	15.355 16.414	1.00 23.74 1.00 20.75	A A
ATOM ATOM	663 664	CD	LYS LYS	87 87	25.231 26.236		17.791 18.627	1.00 19.79 1.00 23.47	A A
ATOM	665	NZ	LYS	87	27.341	29.981	19.117	1.00 25.56	A
ATOM	666		LYS	87	28.131	29.426	20.248	1.00 28.30	A
ATOM	667		LYS	87	24.542	29.479	14.028	1.00 23.80	A
ATOM	668		LYS	87	23.444	29.157	13.557	1.00 23.85	A
ATOM	669		VAL	88	25.708	29.229	13.418	1.00 22.55	A
ATOM	670		VAL	88	25.792	28.439	12.182	1.00 20.90	A
ATOM	671	CB	VAL	88	26.983	28.837	11.263	1.00 18.57	A
ATOM	672	CG1	VAL	88	27.025	27.919	10.055	1.00 17.56	A
ATOM ATOM	673 674	CG2		88 88	26.862 26.094	30.293 27.054	10.823 12.743	1.00 17.32 1.00 20.89	A A
ATOM	675	0	VAL	88	26.995	26.904	13.584	1.00 19.91	A
ATOM	676		VAL	89	25.355	26.047	12.290	1.00 20.24	A
ATOM	677	CA	VAL	89	25.545	24.698	12.807	1.00 20.70	A
ATOM	678		VAL	89	24.282	24.231	13.596	1.00 20.44	A
MOTA	679	CG1		89	24.262	22.783	14.042	1.00 20.44	A

Fig. 2A-11

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Fig. 2A-13

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ATOM
3553 3553 3553 3555 3555 3555 3555 355
CON CABGO O CON CABGO O NA CABGO
ARG ARG ALA ALA ALA ALA LEU LEU LEU LEU LEU LEU LEU ASN ASN ASN
111 111 1112 112 1112 1112 1112 1113 1113 1113 1113 1113 1114 1114
7.016683 9.2284744615887.11666587.12.0089.3199.22897.1666587.11666587.111.00.77801.1111.00.77801.111.00.77801.1111.00.77801.1111.00.77801.1111.00.77
8.441 4.4280 4.0210 7.3473 9.3470 10.3473
1.42000388755134680050778.55566.55566.55566.5578.7778.666.5558.89067709920778.778.8866.558.8906.113.78899920778.89560338875089992078.7889992078.78899992078.78899992078.78899992078.7889999207899999999999999999999999999999
1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
45.27.76.994.0.44.222.222.222.222.23.3.36.23.3.36.22.22.22.22.22.22.22.22.22.22.22.22.22
A A A A A A A A A A A A A A A A A A A

Fig. 2A-15

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ATOM	908	OE2	GLU	118	7.515	13.359	6.798	1.00 38.18	A
ATOM	909	C	GLU	118	9.457	13.174	11.741	1.00 19.53	A
ATOM	910	0	GLU	118	9.253	14.289	12.226	1.00 19.89	A
ATOM	911	N	PHE	119	9.179	12.052	12.397	1.00 16.90	A
ATOM ATOM	912 913	CA CB	PHE PHE	119 119	8.616 8.141	12.072 10.680	13.740 14.123	1.00 14.30 1.00 13.75	A A
ATOM	914	CG	PHE	119	7.379	10.647	15.399	1.00 12.63	A
ATOM	915	CD1	PHE	119	5.987	10.669	15.392	1.00 13.78	A
ATOM	916	CD2	PHE	119	8.046	10.597	16.619	1.00 11.27	A
ATOM	917	CE1	PHE	119	5.271	10.648	16.594	1.00 11.57	A
ATOM ATOM	918 919	CE2 CZ	PHE PHE	119 119	7.345 5.957	10.575 10.599	17.822 17.809	1.00 9.33 1.00 11.88	A A
ATOM	920	C	PHE	119	9.655	12.556	14.754	1.00 12.85	A
MOTA	921	Ö	PHE	119	9.328	13.276	15.692	1.00 12.34	A
MOTA	922	N	ALA	120	10.906	12.147	14.567	1.00 12.61	Α
ATOM	923	CA	ALA	120	12.008	12.554	15.442	1.00 12.28	A
ATOM ATOM	924 925	CB C	ALA ALA	120 120	13.182 12.457	11.624 13.992	15.248 15.155	1.00 8.68 1.00 14.06	A A
ATOM	926	Ö	ALA	120	13.087	14.631	15.133	1.00 14.00	A
MOTA	927	Ň	ILE	121	12.130	14.487	13.961	1.00 15.83	A
MOTA	928	CA	ILE	121	12.510	15.829	13.514	1.00 16.62	A
ATOM	929	CB	ILE	121	12.720	15.820	11.954	1.00 14.14	A
ATOM ATOM	930 931	CG2 CG1	ILE ILE	121 121	12.529 14.126	17.186 15.341	11.357 11.628	1.00 14.79 1.00 13.16	A A
ATOM	932	CD1	ILE	121	15.080	15.491	12.777	1.00 13.15	A
MOTA	933	С	ILE	121	11.499	16.916	13.907	1.00 17.84	A
ATOM	934	0	ILE	121	11.887	18.014	14.333	1.00 18.70	A
ATOM ATOM	935 936	N	ASN	122 122	10.213	16.603 17.537	13.767 14.079	1.00 18.22 1.00 20.53	A A
ATOM	936	CA CB	ASN ASN	122	9.144 9.164	17.927	15.562	1.00 20.33	A
ATOM	938	CG	ASN	122	7.954	18.761	15.967	1.00 18.32	A
ATOM	939	OD1	ASN	122	6.902	18.700	15.333	1.00 15.61	Α
ATOM	940	ND2	ASN	122	8.109	19.550	17.025	1.00 17.45	A
ATOM ATOM	941 942	C 0	ASN ASN	122 122	9.280 9.154	18.784 19.919	13.205 13.684	1.00 23.78 1.00 26.55	A A
ATOM	943	N	GLY	123	9.553	18.564	11.920	1.00 25.65	A
ATOM	944	CA	GLY	123	9.670	19.663	10.969	1.00 25.27	A
MOTA	945	C	GLY	123	10.977	20.428	10.860	1.00 24.57	Α
ATOM	946	0	GLY	123	11.023	21.487	10.243	1.00 24.04	A
ATOM ATOM	947 948	N CA	LEU LEU	124 124	12.043 13.309	19.914 20.607	11.450 11.368	1.00 24.25 1.00 25.19	A A
ATOM	949	CB	LEU	124	13.963	20.703	12.738	1.00 23.50	A
MOTA	950	CG	LEU	124	15.246	21.532	12.711	1.00 22.78	Α
ATOM	951	CD1	LEU	124	15.001	22.839	11.979	1.00 23.39	A
ATOM ATOM	952 953	CD2 C	LEU LEU	124 124	15.701 14.262	21.784 19.924	14.129 10.404	1.00 24.20 1.00 26.33	A A
ATOM	954	Õ	LEU	124	14.865	18.900	10.729	1.00 29.25	Ä
ATOM	955	N	TYR	125	14.383	20.481	9.206	1.00 24.82	A
MOTA	956	CA	TYR	125	15.283	19.923	8.212	1.00 26.15	Α
ATOM	957	CB	TYR	125	14.594	19.748	6.861	1.00 28.22	A
ATOM ATOM	958 959	CG CD1	TYR TYR	125 125	13.328 13.350	18.946 17.555	6.938 6.834	1.00 33.57 1.00 33.93	A A
ATOM	960	CE1	TYR	125	12.184	16.816	6.941	1.00 35.41	A
ATOM	961	CD2	TYR	125	12.102	19.579	7.148	1.00 36.24	Α
MOTA	962	CE2	TYR	125	10.933	18.850	7.257	1.00 36.63	A
MOTA	963	CZ	TYR	125	10.981	17.472	7.153	1.00 37.06	A A
ATOM	964	ОН	TYR	125	9.813	16.759	7.270	1.00 42.14	А

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MOTA	965	С	TYR	125	16.425	20.890	8.056	1.00 23.55	Α
MOTA	966	0	TYR	125	16.323	22.049	8.442	1.00 25.49	Α
ATOM	967	N	PRO	126	17.544	20.417	7.499	1.00 20.61	Α
MOTA	968	CD	PRO	126	17.836	19.054	7.028	1.00 18.09	A
ATOM	969	CA	PRO	126	18.679	21.321	7.319	1.00 17.72	A
ATOM	970	CB	PRO	126	19.759	20.419	6.715	1.00 18.63	A
ATOM	971	CG	PRO	126	19.327	19.012	7.070	1.00 18.55	A
MOTA	972	C	PRO	126	18.293	22.473	6.388	1.00 16.44	A
MOTA	973	0	PRO	126	17.321	22.385	5.643	1.00 16.25	A
MOTA	974	N	ASP	127	19.040	23.565	6.453	1.00 15.85	Α
MOTA	975	CA	ASP	127	18.776	24.695	5.583	1.00 16.90	A
MOTA	976	CB	ASP	127	19.154	26.002	6.279	1.00 18.60	A
MOTA	977	CG	ASP	127	17.970	26.642	6.984	1.00 21.07	Α
MOTA	978	OD1		127	16.959	26.964	6.306	1.00 22.71	A
MOTA	979		ASP	127	18.047	26.820	8.219	1.00 18.29	A
MOTA	980	C	ASP	127	19.613	24.491	4.324	1.00 18.15	A
ATOM	981	0	ASP	127	19.393	25.151	3.310	1.00 19.18	A
MOTA	982	N	LEU	128	20.567	23.557	4.413	1.00 18.37	A
ATOM	983	CA	LEU	128	21.469	23.185	3.318	1.00 16.53	A
MOTA	984 985	CB	LEU	128	22.523	24.286	3.079 2.236	1.00 15.81	A
ATOM ATOM	986	CG CD1	LEU LEU	128 128	23.762	23.924	0.764	1.00 14.34	A
ATOM	987			128	23.384 24.919	23.972 24.858	2.515	1.00 16.21 1.00 8.51	A A
ATOM	988	CDZ	LEU	128	22.174	21.884	3.707	1.00 16.96	A
ATOM	989	Ö	LEU	128	22.682	21.771	4.818	1.00 10.90	Ā
ATOM	990	N	THR	129	22.200	20.905	2.800	1.00 17.03	A
ATOM	991	CA	THR	129	22.861	19.614	3.062	1.00 19.58	A
ATOM	992	CB	THR	129	21.870	18.429	2.981	1.00 19.13	A
ATOM	993	OG1	THR	129	21.084	18.375	4.178	1.00 21.93	A
ATOM	994	CG2	THR	129	22.623	17.116	2.826	1.00 18.43	A
ATOM	995	С	THR	129	23.955	19.381	2.026	1.00 18.88	A
MOTA	996	0	THR	129	23.665	19.248	0.837	1.00 19.90	Α
MOTA	997	N	ILE	130	25.204	19.317	2.472	1.00 17.60	A
ATOM	998	CA	ILE	130	26.334	19.119	1.561	1.00 16.04	А
ATOM	999	CB	ILE	130	27.640	19.749	2.148	1.00 16.79	A
ATOM	1000	CG2	ILE	130	28.863	19.240	1.382	1.00 17.88	A
ATOM	1001	CG1	ILE	130	27.563	21.283	2.111	1.00 17.22	A
ATOM	1002	CD1	ILE	130	27.946	21.898	0.759	1.00 15.20	A
ATOM	1003	C	ILE	130	26.591	17.638	1.289	1.00 14.63	A
ATOM ATOM	1004 1005	O N	ILE TYR	130 131	27.029 26.327	16.916 17.187	2.169 0.072	1.00 13.93 1.00 13.78	A A
ATOM	1005	CA	TYR	131	26.568	15.796	-0.261	1.00 13.78	A
ATOM	1007	CB	TYR	131	25.462	15.258	-1.156	1.00 14.00	A
ATOM	1008	CG	TYR	131	25.706	13.816	-1.517	1.00 18.24	A
ATOM	1009	CD1	TYR	131	25.470	12.811	-0.592	1.00 19.69	A
ATOM	1010	CE1	TYR	131	25.728	11.480	-0.893	1.00 20.72	A
ATOM	1011	CD2	TYR	131	26.210	13.457	-2.770	1.00 20.82	A
MOTA	1012	CE2	TYR	131	26.471	12.123	-3.083	1.00 20.33	A
ATOM .	1013	CZ	TYR	131	26.226	11.141	-2.133	1.00 20.01	A
MOTA	1014	OH	TYR	131	26.484	9.821	-2.407	1.00 22.90	Α
MOTA	1015	C	TYR	131	27.919	15.559	-0.948	1.00 13.59	Α
MOTA	1016	0	TYR	131	28.117	15.869	-2.124	1.00 13.47	Α
ATOM	1017	N	LEU	132	28.851	15.005	-0.198	1.00 12.69	A
ATOM	1018	CA	LEU	132	30.158	14.712	-0.736	1.00 14.00	A
ATOM	1019	CB	LEU	132	31.146	14.463	0.405	1.00 10.84	A
ATOM	1020	CG CD1	LEU	132	31.323	15.688	1.306	1.00 11.12	A
MOTA	1021	CDI	LEU	132	32.263	15.370	2.455	1.00 15.11	A

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ATOM 1022 CD2 LEU 132 31.883 16.845 0.487 1.00 10.94 A ATOM 1023 C LEU 132 30.033 13.489 -1.638 1.00 16.10 A ATOM 1024 O LEU 132 30.097 12.337 -1.186 1.00 15.70 A ATOM 1025 N ASN 133 29.823 13.766 -2.920 1.00 16.64 A ATOM 1026 CA ASN 133 29.679 12.745 -3.955 1.00 16.26 A ATOM 1027 CB ASN 133 29.146 13.401 -5.222 1.00 15.66 A ATOM 1028 CG ASN 133 28.209 12.515 -5.977 1.00 15.86 A ATOM 1029 OD1 ASN 133 28.399 11.303 -6.033 1.00 19.55 A ATOM 1030 ND2 ASN 133 27.178 13.105 -6.662 1.00 18.53 A ATOM 1031 C ASN 133 30.986 12.006 -4.289 1.00 16.44 A ATOM 1032 O ASN 133 31.804 12.495 -5.070 1.00 16.93 A ATOM 1033 N VAL 134 31.174 10.822 -3.711 1.00 14.84 A ATOM 1034 CA VAL 134 32.376 10.026 -3.959 1.00 13.84 A ATOM 1036 CG1 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1037 CG2 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1038 C VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1039 O VAL 134 31.000 8.711 1.00 15.51 A ATOM 1039 C VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 15.03 A ATOM 1041 CA SER 135 32.868 8.290 -5.618 1.00 15.07 A ATOM 1042 CB SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1044 C SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1044 C SER 135 33.284 7.059 -6.348 1.00 15.07 A ATOM 1047 CA ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.422 4.745 -5.703 1.00 15.08 A
ATOM 1026 CA ASN 133 29.679 12.745 -3.955 1.00 16.26 A ATOM 1027 CB ASN 133 29.146 13.401 -5.222 1.00 15.66 A ATOM 1028 CG ASN 133 28.209 12.515 -5.977 1.00 15.86 A ATOM 1029 OD1 ASN 133 28.399 11.303 -6.033 1.00 19.55 A ATOM 1030 ND2 ASN 133 27.178 13.105 -6.562 1.00 18.53 A ATOM 1031 C ASN 133 30.986 12.006 -4.289 1.00 16.44 A ATOM 1032 O ASN 133 31.804 12.495 -5.070 1.00 16.93 A ATOM 1033 N VAL 134 31.174 10.822 -3.711 1.00 14.84 A ATOM 1034 CA VAL 134 32.376 10.026 -3.959 1.00 15.03 A ATOM 1035 CB VAL 134 32.376 10.026 -3.959 1.00 15.03 A ATOM 1036 CGI VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1037 CG2 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1038 C VAL 134 32.027 8.723 -4.679 1.00 16.69 A ATOM 1039 O VAL 134 31.000 8.8111 -4.386 1.00 17.63 A ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 17.63 A ATOM 1040 CB SER 135 32.868 8.290 -5.618 1.00 15.37 A ATOM 1040 CB SER 135 32.868 8.290 -5.618 1.00 15.37 A ATOM 1040 C SER 135 33.284 7.059 -6.348 1.00 15.37 A ATOM 1040 C SER 135 33.284 7.059 -6.348 1.00 15.13 A ATOM 1040 C SER 135 33.284 7.059 -6.348 1.00 15.37 A ATOM 1044 C SER 135 33.286 6.860 -7.562 1.00 19.69 A ATOM 1045 O SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.422 4.745 -5.703 1.00 15.08 A
ATOM 1028 CG ASN 133 28.209 12.515 -5.977 1.00 15.86 A ATOM 1029 OD1 ASN 133 28.399 11.303 -6.033 1.00 19.55 A ATOM 1030 ND2 ASN 133 27.178 13.105 -6.562 1.00 18.53 A ATOM 1031 C ASN 133 30.986 12.006 -4.289 1.00 16.44 A ATOM 1032 O ASN 133 31.804 12.495 -5.070 1.00 16.93 A ATOM 1033 N VAL 134 31.174 10.822 -3.711 1.00 14.84 A ATOM 1034 CA VAL 134 32.376 10.026 -3.959 1.00 15.03 A ATOM 1035 CB VAL 134 32.376 10.026 -3.959 1.00 15.03 A ATOM 1036 CG1 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1037 CG2 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1038 C VAL 134 34.591 9.738 -2.850 1.00 12.76 A ATOM 1038 C VAL 134 32.027 8.723 -4.679 1.00 16.69 A ATOM 1039 O VAL 134 31.000 8.111 -4.386 1.00 17.63 A ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 15.37 A ATOM 1041 CA SER 135 32.868 8.290 -5.618 1.00 15.37 A ATOM 1042 CB SER 135 33.284 7.059 -6.348 1.00 15.37 A ATOM 1044 C SER 135 33.284 7.059 -6.348 1.00 15.13 A ATOM 1044 C SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1044 C SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1045 O SER 135 34.680 6.894 -5.530 1.00 15.42 A ATOM 1045 O SER 135 34.021 6.034 -4.761 1.00 16.48 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.422 4.745 -5.703 1.00 15.08 A
ATOM 1030 ND2 ASN 133 27.178 13.105 -6.562 1.00 18.53 A ATOM 1031 C ASN 133 30.986 12.006 -4.289 1.00 16.44 A ATOM 1032 O ASN 133 31.804 12.495 -5.070 1.00 16.93 A ATOM 1033 N VAL 134 31.174 10.822 -3.711 1.00 14.84 A ATOM 1034 CA VAL 134 32.376 10.026 -3.959 1.00 15.03 A ATOM 1035 CB VAL 134 33.093 9.689 -2.642 1.00 13.84 A ATOM 1036 CG1 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1037 CG2 VAL 134 34.591 9.738 -2.850 1.00 12.76 A ATOM 1038 C VAL 134 32.027 8.723 -4.679 1.00 16.69 A ATOM 1039 O VAL 134 31.000 8.111 -4.386 1.00 17.63 A ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 15.07 A ATOM 1041 CA SER 135 32.584 7.059 -6.348 1.00 15.37 A ATOM 1042 CB SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1043 OG SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1044 C SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1044 C SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1045 O SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69
ATOM 1032 O ASN 133 31.804 12.495 -5.070 1.00 16.93 A ATOM 1033 N VAL 134 31.174 10.822 -3.711 1.00 14.84 A A ATOM 1034 CA VAL 134 32.376 10.026 -3.959 1.00 15.03 A ATOM 1035 CB VAL 134 33.093 9.689 -2.642 1.00 13.84 A A ATOM 1036 CG1 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1037 CG2 VAL 134 34.591 9.738 -2.850 1.00 12.76 A ATOM 1038 C VAL 134 32.027 8.723 -4.679 1.00 16.69 A ATOM 1039 O VAL 134 31.000 8.111 -4.386 1.00 17.63 A ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 15.07 A ATOM 1041 CA SER 135 32.868 8.290 -5.618 1.00 15.37 A ATOM 1042 CB SER 135 33.284 7.059 -6.348 1.00 15.37 A ATOM 1042 CB SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1043 OG SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1044 C SER 135 33.069 5.894 -5.530 1.00 15.42 A ATOM 1045 O SER 135 34.021 6.034 -4.761 1.00 16.48 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69
ATOM 1034 CA VAL 134 32.376 10.026 -3.959 1.00 15.03 A ATOM 1035 CB VAL 134 33.093 9.689 -2.642 1.00 13.84 A ATOM 1036 CG1 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1037 CG2 VAL 134 34.591 9.738 -2.850 1.00 12.76 A ATOM 1038 C VAL 134 32.027 8.723 -4.679 1.00 16.69 A ATOM 1039 O VAL 134 31.000 8.111 -4.386 1.00 17.63 A ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 15.07 A ATOM 1041 CA SER 135 32.868 8.290 -5.618 1.00 15.37 A ATOM 1042 CB SER 135 33.284 7.059 -6.348 1.00 15.37 A ATOM 1043 OG SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1044 C SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1045 O SER 135 34.021 6.034 -4.761 1.00 16.48 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69
ATOM 1036 CG1 VAL 134 32.673 8.311 -2.147 1.00 15.51 A ATOM 1037 CG2 VAL 134 34.591 9.738 -2.850 1.00 12.76 A ATOM 1038 C VAL 134 32.027 8.723 -4.679 1.00 16.69 A ATOM 1039 O VAL 134 31.000 8.111 -4.386 1.00 17.63 A ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 15.07 A ATOM 1041 CA SER 135 32.584 7.059 -6.348 1.00 15.37 A ATOM 1042 CB SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1043 OG SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1044 C SER 135 33.069 5.894 -5.530 1.00 15.42 A ATOM 1045 O SER 135 34.021 6.034 -4.761 1.00 16.48 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69
ATOM 1038 C VAL 134 32.027 8.723 -4.679 1.00 16.69 A ATOM 1039 O VAL 134 31.000 8.111 -4.386 1.00 17.63 A ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 15.07 A ATOM 1041 CA SER 135 32.584 7.059 -6.348 1.00 15.37 A ATOM 1042 CB SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1043 OG SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1044 C SER 135 33.069 5.894 -5.530 1.00 15.42 A ATOM 1045 O SER 135 34.021 6.034 -4.761 1.00 16.48 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69
ATOM 1040 N SER 135 32.868 8.290 -5.618 1.00 15.07 A ATOM 1041 CA SER 135 32.584 7.059 -6.348 1.00 15.37 A ATOM 1042 CB SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1043 OG SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1044 C SER 135 33.069 5.894 -5.530 1.00 15.42 A ATOM 1045 O SER 135 34.021 6.034 -4.761 1.00 16.48 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69
ATOM 1042 CB SER 135 33.284 7.051 -7.711 1.00 15.13 A ATOM 1043 OG SER 135 34.680 6.860 -7.562 1.00 19.69 A ATOM 1044 C SER 135 33.069 5.894 -5.530 1.00 15.42 A ATOM 1045 O SER 135 34.021 6.034 -4.761 1.00 16.48 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69 A
ATOM 1044 C SER 135 33.069 5.894 -5.530 1.00 15.42 A ATOM 1045 O SER 135 34.021 6.034 -4.761 1.00 16.48 A ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69 A
ATOM 1046 N ALA 136 32.422 4.745 -5.703 1.00 15.08 A ATOM 1047 CA ALA 136 32.785 3.539 -4.973 1.00 15.69 A
ATOM 1048 CB ALA 136 32.012 2.351 -5.517 1.00 13.23 A
ATOM 1049 C ALA 136 34.282 3.232 -4.982 1.00 16.27 A ATOM 1050 O ALA 136 34.835 2.849 -3.940 1.00 17.62 A
ATOM 1051 N GLU 137 34.936 3.417 -6.136 1.00 16.13 A ATOM 1052 CA GLU 137 36.373 3.128 -6.295 1.00 16.92 A
ATOM 1053 CB GLU 137 36.769 3.211 -7.761 1.00 19.08 A ATOM 1054 CG GLU 137 36.099 2.193 -8.627 1.00 21.24 A
ATOM 1055 CD GLU 137 34.697 2.606 -9.026 1.00 26.03 A ATOM 1056 OE1 GLU 137 34.254 3.703 -8.607 1.00 26.26 A
ATOM 1057 OE2 GLU 137 34.050 1.830 -9.762 1.00 24.36 A ATOM 1058 C GLU 137 37.329 4.010 -5.519 1.00 17.18 A
ATOM 1059 O GLU 137 38.293 3.529 -4.914 1.00 18.42 A ATOM 1060 N VAL 138 37.102 5.315 -5.592 1.00 16.65 A
ATOM 1061 CA VAL 138 37.930 6.286 -4.880 1.00 13.99 A ATOM 1062 CB VAL 138 37.571 7.729 -5.317 1.00 12.36 A
ATOM 1063 CG1 VAL 138 38.315 8.722 -4.480 1.00 7.64 A ATOM 1064 CG2 VAL 138 37.876 7.909 -6.812 1.00 11.17 A
ATOM 1065 C VAL 138 37.650 6.107 -3.388 1.00 12.75 A ATOM 1066 O VAL 138 38.566 6.069 -2.577 1.00 12.84 A
ATOM 1067 N GLY 139 36.372 5.979 -3.040 1.00 12.35 A ATOM 1068 CA GLY 139 35.998 5.790 -1.650 1.00 13.46 A
ATOM 1069 C GLY 139 36.696 4.593 -1.031 1.00 12.84 A ATOM 1070 O GLY 139 37.247 4.681 0.071 1.00 11.91 A
ATOM 1071 N ARG 140 36.675 3.469 -1.743 1.00 14.34 A ATOM 1072 CA ARG 140 37.314 2.239 -1.268 1.00 15.31 A
ATOM 1073 CB ARG 140 37.279 1.164 -2.357 1.00 14.32 A ATOM 1074 CG ARG 140 38.142 -0.052 -2.045 1.00 13.59 A
ATOM 1075 CD ARG 140 38.881 -0.509 -3.270 1.00 15.36 A ATOM 1076 NE ARG 140 38.006 -0.522 -4.439 1.00 16.56 A
ATOM 1077 CZ ARG 140 38.406 -0.294 -5.685 1.00 14.11 A ATOM 1078 NH1 ARG 140 39.684 -0.029 -5.942 1.00 10.53 A

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1079 1081 1082 1083 1084 1088 1088 1088 1088 1099 1109 1109 1109	C O N CA CB CCD O N CA CB CCD C O N CA CB CCD C O N CA CB CCD C O N CA CB CCD C C O N CA CB CCD C C C C C C C C C C C C C C C C	ARG ARG ILE	1400 1411 1411 1411 1411 1411 1411 1411	37.562 38.179 39.526 41.464 41.996 41.469 41.469 41.257 39.623 40.421 42.257 38.328 40.421 39.623	3.264 1.850 0.894 1.678 4.131 3.915 5.057 7.137 8.047 9.932 10.835 11.417 15.301 4.332 3.568 2.621 1.480 3.389 2.7736 2.235 1.490 -0.149 -0.149 -0.149 -2.180 -4.059 -2.187 -6.059 -7.6663 -9.789 -9.789	-6.678 -0.2839 -1.8651 -2.8759 -1.8799 -1.3.3891 -1.01256 -0.33591 -0.3559 -1.3827 -1.3827 -1.3827 -1.3829	1.00 10.78 1.00 17.87 1.00 18.73 1.00 18.85 1.00 19.21 1.00 19.92 1.00 20.18 1.00 23.75 1.00 25.20 1.00 23.49 1.00 22.21 1.00 24.64 1.00 22.42 1.00 20.34 1.00 20.34 1.00 20.93 1.00 20.53 1.00 17.90 1.00 14.20 1.00 19.58 1.00 22.51 1.00 23.25 1.00 23.18 1.00 22.51 1.00 23.25 1.00 23.18 1.00 22.70 1.00 23.25 1.00 23.18 1.00 22.70 1.00 23.25 1.00 25.38 1.00 27.37 1.00 25.38 1.00 27.49 1.00 28.27 1.00 27.49 1.00 28.27 1.00 27.56 1.00 27.68 1.00 27.56 1.00 27.56 1.00 27.68 1.00 27.56 1.00 51.95 1.00 51.95 1.00 51.95 1.00 51.95 1.00 51.95 1.00 53.96 1.00 53.96 1.00 53.96 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.30 1.00 53.35	AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
ATOM ATOM ATOM	1127 1128 1129	CA CB CG	GLN GLN GLN	155 155 155	36.277 36.743 38.116	-7.663 -9.086 -9.461 -9.789 -9.959 -9.882 -7.555 -6.458	0.251 0.590 0.005	1.00 51.32 1.00 52.85 1.00 56.38	A A A

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1136 1137 1138 1140 1141 1142 1143 1144 1145 1145 1155 1155 1155 1156 1166 116	CA GLU CB GLU CG GLU OE1 GLU OE2 GLU OE2 GLU O GLU N ASP CB ASP CB ASP OD1 ASP CD ASP OD2 ASP OD2 ASP OD2 ASP CD LEU CD LEU CD LEU CD LEU CD LYS CD LYS CD LYS CD LYS CD LYS CD LYS CD CD N CA CB CD C	$\begin{array}{c} 1556666666777777788888888899999999990000000000$	32.563 32.044 32.365 33.512 34.663 31.909 30.7886 32.283 33.7820 32.1820 32.18	-8.684 -10.108 -11.046 -10.522 -10.931 -9.692 -7.405 -6.309 -7.2290 -6.3087 -8.3253 -4.8890 -7.683 -8.3253 -4.8890 -3.8868 -4.896 -2.4453 -2.4453 -5.7044 -5.7745 -5.6702 -3.4666 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.4643 -2.6	0.211 0.439 -0.713 -1.559 -1.304 -2.463 1.199 1.088 2.165 4.400 4.647 3.823 5.678 2.5201 1.197 0.445 -1.537 -1.4537 -1.4537 -1.4537 -1.4516 -1.516 -1.516 -1.644 -2.644 -2.644 -2.644 -2.644 -2.644 -2.644 -2.644 -2.644 -2.644 -2.644 -2.644 -2.644 -2.644 -3.644 -3.645 -1.64	1.00 47.47 1.00 49.49 1.00 52.78 1.00 55.94 1.00 56.30 1.00 45.09 1.00 44.40 1.00 45.02 1.00 42.71 1.00 44.86 1.00 45.91 1.00 46.98 1.00 46.41 1.00 39.90 1.00 39.56 1.00 32.56 1.00 32.56 1.00 34.63 1.00 29.36 1.00 29.36 1.00 29.36 1.00 29.36 1.00 29.36 1.00 27.62 1.00 30.02 1.00 33.24 1.00 26.45 1.00 23.70 1.00 26.45 1.00 23.70 1.00 26.99 1.00 27.62 1.00 33.24 1.00 35.50 1.00 21.27 1.00 16.96 1.00 19.06 1.00 19.06 1.00 19.06 1.00 19.06	A A A A A A A A A A A A A A A A A A A
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1169 1170 1171 1172 1173 1174 1175 1176	N PHE CA PHE CB PHE CG PHE CD1 PHE CD2 PHE CE1 PHE CE2 PHE	160 160 160 160 160 160 160	28.282 27.406 27.769 26.905 25.561 27.453 24.774 26.678	-3.304 -2.480 -2.642 -1.833 -2.147 -0.780 -1.427 -0.053	0.837 1.664 3.145 4.091 4.284 4.827 5.208 5.750	1.00 20.82 1.00 21.15 1.00 18.20 1.00 18.88 1.00 17.68 1.00 19.06 1.00 18.90 1.00 19.17	A A A A A A
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1179 1180 1181 1182 1183 1184 1185 1186 1187 1188 1189	O PHE N HIS CA HIS CB HIS CG HIS CD2 HIS ND1 HIS CE1 HIS NE2 HIS C HIS O HIS	160 161 161 161 161 161 161 161	26.653 28.874 29.243 30.759 31.419 30.933 32.776 33.071 31.982 28.700 28.241	-0.322 -0.595 0.766 0.928 0.384 -0.316 0.550 -0.023 -0.559 1.125 2.240	0.888 1.204 0.802 0.787 2.000 3.049 2.256 3.396 3.908 -0.564 -0.773 -1.504	1.00 23.35 1.00 24.22 1.00 25.47 1.00 27.63 1.00 32.09 1.00 34.82 1.00 34.79 1.00 36.30 1.00 36.79 1.00 24.44 1.00 25.74 1.00 22.83	A A A A A A A A
ATOM ATOM ATOM	1190 1191 1192	N GLU CA GLU CB GLU	162 162 162	28.756 28.241 28.703	0.192 0.474 -0.600	-2.830 -3.818	1.00 22.65 1.00 23.31	A A A

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ATOM ATOM ATOM ATOM	1193 1194 1195 1196	CG GLU CD GLU OE1 GLU OE2 GLU	162 162 162 162	27.748 28.170 27.343 29.341	-1.770 -2.730 -3.049 -3.163	-3.975 -5.082 -5.969 -5.062	1.00 28.61 1.00 30.31 1.00 26.26 1.00 33.07	A A A
OM OM OM OM OM OM OM	1197 1198 1199 1200 1201 1202 1203	C GLU O GLU N LYS CA LYS CB LYS CG LYS CD LYS	162 163 163 163 163 163	26.718 26.085 26.137 24.684 24.277 22.849 22.742	0.545 1.159 -0.076 -0.089 -1.234 -1.705 -3.203	-2.769 -3.624 -1.744 -1.549 -0.624 -0.818 -0.585	1.00 22.17 1.00 22.37 1.00 21.89 1.00 21.28 1.00 24.16 1.00 27.09 1.00 28.27	A A A A A
i I I I I	1204 1205 1206 1207 1208 1209	CE LYS NZ LYS C LYS O LYS N VAL CA VAL	163 163 163 163 164 164	21.319 20.331 24.231 23.147 25.080 24.835	-3.703 -2.614 1.218 1.739 1.721 2.973	-0.793 -1.060 -0.923 -1.216 -0.032 0.661	1.00 31.58 1.00 32.32 1.00 21.34 1.00 16.85 1.00 21.65 1.00 20.57	A A A A A
1 4 4 4 4 4	1210 1211 1212 1213 1214 1215	CB VAL CG1 VAL CG2 VAL C VAL O VAL N ILE	164 164 164 164 164 165	25.982 25.949 25.892 24.797 23.862 25.845	3.301 4.796 2.418 4.075 4.880 4.105	1.637 1.986 2.879 -0.386 -0.432 -1.206	1.00 20.82 1.00 20.62 1.00 14.98 1.00 20.01 1.00 18.78 1.00 20.78	A A A A A
M M M M M	1216 1217 1218 1219 1220 1221	CA ILE CB ILE CG2 ILE CG1 ILE CD1 ILE C ILE	165 165 165 165 165 165	25.985 27.198 27.160 28.487 29.739 24.716	5.092 4.782 5.633 5.086 4.834 5.118	-2.261 -3.149 -4.397 -2.389 -3.191 -3.099	1.00 20.28 1.00 19.12 1.00 21.64 1.00 17.77 1.00 17.87 1.00 22.78	A A A A A
M OM OM OM OM OM	1222 1223 1224 1225 1226 1227	O ILE N GLU CA GLU CB GLU CG GLU CD GLU	165 166 166 166 166 166	24.224 24.176 22.939 22.584 23.712 23.230	6.188 3.937 3.827 2.356 1.483 0.093	-3.459 -3.387 -4.159 -4.376 -4.893 -5.321	1.00 23.05 1.00 24.97 1.00 27.18 1.00 31.42 1.00 37.18 1.00 41.68	A A A A A
M M M M M	1228 1229 1230 1231 1232 1233	OE1 GLU OE2 GLU C GLU O GLU N GLY CA GLY	166 166 166 166 167 167	24.027 22.053 21.750 20.922 21.657 20.567	-0.659 -0.250 4.521 5.151 4.383 5.013	-5.932 -5.044 -3.466 -4.125 -2.144 -1.409	1.00 41.28 1.00 42.53 1.00 27.12 1.00 26.40 1.00 26.20 1.00 23.21	A A A A A
MC MC MC OM OM OM OM	1234	C GLY O GLY N TYR CA TYR CB TYR CG TYR	167 167 168 168 168 168	20.675 19.678 21.910 22.206 23.694 24.031	6.524 7.245 6.995 8.415 8.594 8.806	-1.384 -1.429 -1.315 -1.302 -1.044 0.404	1.00 20.91	A A A A A
OM OM OM OM OM	1240 1241 1242 1243 1244	CD1 TYR CE1 TYR CD2 TYR CE2 TYR CZ TYR	168 168 168 168 168	25.071 25.424 23.345 23.683 24.725	8.109 8.352 9.748 10.004 9.305	1.008 2.332 1.160 2.489 3.072	1.00 17.79 1.00 20.01 1.00 19.07 1.00 18.60 1.00 20.26	A A A A
OM OM OM OM OM	1245 1246 1247 1248 1249	OH TYR C TYR O TYR N GLN CA GLN	168 168 168 169 169	25.067 21.810 21.275 22.078 21.740	9.563 9.070 10.179 8.380 8.884	4.382 -2.632 -2.650 -3.741 -5.070	1.00 21.55 1.00 23.66 1.00 26.01 1.00 25.06 1.00 25.35	A A A A

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ATOM	1250	СВ	GLN	169	22.184	7.905	-6.155	1.00 26.00	А
ATOM ATOM	1251 1252	CG CD	GLN GLN	169 169	23.626 24.615	7.463 8.593	-6.053 -6.299	1.00 29.17 1.00 29.94	A A
MOTA	1253	OE1	GLN	169	25.820	8.429	-6.095	1.00 29.50	A
ATOM ATOM	1254 1255	NE2 C	GLN	169 169	24.108 20.239	9.749 9.066	-6.737 -5.187	1.00 28.14 1.00 26.60	A A
ATOM	1256	Ö	GLN	169	19.767	10.051	-5.738	1.00 27.89	A
MOTA	1257	N	GLU	170	19.494	8.098	-4.671	1.00 26.92	A
ATOM ATOM	1258 1259	CA CB	GLU GLU	170 170	18.040 17.468	8.143 6.844	-4.714 -4.171	1.00 28.01 1.00 29.99	A A
MOTA	1260	CG	GLU	170	16.121	6.500	-4.744	1.00 35.53	A
ATOM ATOM	1261 1262	CD OE1	GLU GLU	170 170	16.204 15.566	5.361 4.317	-5.728 -5.483	1.00 39.43 1.00 42.68	A A
ATOM	1263	OE2	GLU	170	16.912	5.506	-6.748	1.00 42.38	A
ATOM ATOM	1264 1265	C	GLU GLU	170 170	17.501 16.591	9.302 10.012	-3.892 -4.319	1.00 27.62 1.00 26.01	A A
ATOM	1266	O N	ILE	171	18.075	9.476	-2.703	1.00 28.74	A
MOTA	1267	CA	ILE	171	17.682	10.536	-1.780	1.00 27.14	A
ATOM ATOM	1268 1269	CB CG2	ILE ILE	171 171	18.521 18.247	10.483 11.703	-0.499 0.342	1.00 26.26 1.00 26.85	A A
MOTA	1270	CG1	ILE	171	18.202	9.215	0.287	1.00 25.90	Α
ATOM ATOM	1271 1272	CD1 C	ILE ILE	171 171	19.322 17.879	8.780 11.906	1.191 -2.410	1.00 25.67 1.00 28.17	A A
MOTA	1273	0	ILE	171	16.912	12.641	-2.637	1.00 28.24	Α
ATOM ATOM	1274 1275	N CA	ILE ILE	172 172	19.139 19.495	12.244 13.520	-2.680 -3.291	1.00 27.45 1.00 25.70	A A
ATOM	1276	CB	ILE	172	21.019	13.624	-3.504	1.00 26.14	A
ATOM ATOM	1277 1278	CG2	ILE	172 172	21.749	13.012	-2.326 -4.790	1.00 24.71 1.00 29.17	A
ATOM	1278	CG1 CD1	ILE ILE	172	21.415 22.906	12.889 12.768	-4.790 -5.016	1.00 29.17 1.00 28.48	A A
ATOM	1280	C	ILE	172	18.797	13.657	-4.639	1.00 24.52	Α
ATOM ATOM	1281 1282	O N	ILE PHE	172 179	18.259 19.876	14.715 19.984	-4.963 -2.975	1.00 26.19 1.00 42.30	A A
MOTA	1283	CA	PHE	179	21.092	19.709	-2.209	1.00 38.28	Α
ATOM ATOM	1284 1285	CB CG	PHE PHE	179 179	21.397 20.373	18.199 17.380	-2.157 -1.412	1.00 36.78 1.00 34.19	A A
MOTA	1286	CD1	PHE	179	19.165	17.052	-2.012	1.00 33.67	Α
ATOM ATOM	1287 1288	CD2 CE1	PHE PHE	179 179	20.634 18.229	16.909 16.263	-0.129 -1.347	1.00 31.49 1.00 33.59	A A
ATOM	1289	CE2	PHE	179	19.707	16.121	0.543	1.00 32.04	A
ATOM ATOM	1290 1291	CZ C	PHE PHE	179 179	18.500 22.231	15.797 20.384	-0.067 -2.937	1.00 32.17 1.00 36.53	A A
ATOM	1292	Ö	PHE	179	22.231	21.059	-3.950	1.00 30.33	A
ATOM	1293	N	LYS	180	23.433	20.178	-2.417	1.00 34.55	Α
ATOM ATOM	1294 1295	CA CB	LYS LYS	180 180	24.644 25.148	20.711 21.909	-3.003 -2.194	1.00 32.09 1.00 33.81	A A
MOTA	1296	CG	LYS	180	24.267	23.151	-2.328	1.00 35.25	Α
ATOM ATOM	1297 1298	CD CE	LYS LYS	180 180	23.799 22.706	23.308 24.354	-3.767 -3.928	1.00 37.60 1.00 40.95	A A
ATOM	1299	NZ	LYS	180	22.097	24.264	-5.300	1.00 42.21	Α
ATOM ATOM	1300 1301	C 0	LYS LYS	180 180	25.642 26.255	19.565 19.286	-2.959 -1.925	1.00 31.09 1.00 29.48	A A
MOTA	1302	N	SER	181	25.775	18.874	-4.083	1.00 30.63	A
ATOM ATOM	1303 1304	CA CB	SER SER	181 181	26.695 26.248	17.760 16.771	-4.157 -5.234	1.00 30.95 1.00 31.00	A A
MOTA	1305	OG	SER	181	27.097	16.850	-6.360	1.00 35.32	Α
ATOM	1306	С	SER	181	28.077	18.287	-4.485	1.00 30.42	A

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
1307 1308 1309 13112 13113 13115 131
CB CG2 CG ON CA CB CG ODD2 CON CA CB CG CD NEC CON CA CB CG CD NEC CON CA CB CG CD NEC C
SERL VALL VALL VASN ASN AALA ALA ASPPPPROODO GEN PROODO PROOD PRODUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUUU
181 182 182 182 183 183 183 183 183 184 184 185 185 185 185 186 186 186 187 177 187 188 188 188 188 188 188 188
28.203 29.0473 30.4756 30.5216 30.5
19.753 18.79308 19.7432 18.79308 18.79308 16.715.30918 17.19309 16.715.30918 17.19309 17.19309 17.19309 18.19309 1
-5.80303 -2.91583 -4.191583 -2.91583 -5.40207 -6.30622 -4.16030692 -7.30622 -7.3073 -7
1.00 29.79 1.00 29.85 1.00 29.85 1.00 30.06 1.00 27.74 1.00 24.75 1.00 27.76 1.00 28.79 1.00 29.95 1.00 30.78 1.00 29.79 1.00 30.37 1.00 30.37 1.00 32.12 1.00 32.12 1.00 32.12 1.00 33.21 1.00 35.05 1.00 37.72 1.00 37.58 1.00 37.72 1.00 33.88 1.00 37.72 1.00 33.88 1.00 33.12 1.00 33.88 1.00 33.12 1.00 33.12 1.00 33.12 1.00 33.12 1.00 33.15 1.00 33.15 1.00 35.39 1.00 35.39 1.00 37.46 1.00 37.46 1.00 37.46 1.00 37.46 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.35 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38 1.00 39.38
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Fig. 2A-23

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
142234456789012234425678901141111111111111111111111111111111111
CD2 TYR CE2 TYR CE2 TYR CE3 TYR CE4 TYR CE5 TYR CE5 TYR CE6 TYR CE7 CA CHAR CE8 CHAR CE8 CHAR CE8 THR CE8 THR CE8 THR CE8 THR CE9 TYR
196 196 196 197 197 197 197 197 197 198 198 198 198 199 199 199 199 199 199
35.972 36.142 35.715 35.876 32.922 31.953 33.331 32.664 33.244 34.741 35.117 36.263 34.152 30.381 30.790 29.381 29.747 27.711 28.641 27.489 29.306 29.491 29.306 29.491 29.748 31.133 31.860 27.906 27.907 27.906 27.906 27.906 27.906 27.906 27.906 27.906 27.906 27.907 27.906 27.907 27.906 27.907 27.906 27.906 27.906 27.906 27.906 27.906 27.906 27.906 27.907 27.906 27
29.011 30.247 30.421 31.642 27.770 27.409 28.367 29.28.307 28.367 29.28.307 28.307 28.307 28.4557 29.368.457 27.367 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.3777 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.3777 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.3777 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.3777 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.3777 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.3777 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.3777 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.377 27.3777 27.377 27.37777 27.3777 27.3777 27.3777 27.3777 27.3777 27.3777 27.3777 27.37777 27.37777 27.3777 27.3777 27.3777 27.3777 27.3777 27.3777 27.3777 27
1.666 2.2837 4.2807 1.3268 0.807 1.3268 -2.8998 0.426 -2.8298 -2.8298 -1.3997 -1.428 -2.1825 -1.4700 -1.3263 -1.4700 -1.2748 -1.5248 -1.5428 -1.5428 -1.3476 -1.3428 -
1.00 29.95 1.00 30.27 1.00 32.29 1.00 28.75 1.00 28.74 1.00 29.70 1.00 30.12 1.00 34.57 1.00 34.65 1.00 36.28 1.00 29.67 1.00 30.98 1.00 29.67 1.00 30.01 1.00 31.23 1.00 29.67 1.00 29.60 1.00 29.60 1.00 29.22 1.00 26.89 1.00 29.22 1.00 26.49 1.00 24.49 1.00 24.49 1.00 24.49 1.00 24.49 1.00 24.95 1.00 26.20 1.00 26.20 1.00 27.38 1.00 29.81 1.00 29.81 1.00 29.81 1.00 29.81 1.00 29.81 1.00 29.81 1.00 29.81 1.00 31.60 1.00 35.63 1.00 35.63 1.00 37.00 1.00 35.63 1.00 37.00 1.00 37.00 1.00 37.00 1.00 38.46 1.00 39.22 1.00 39.22
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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
1479 1481 1482 1488 1488 1488 1488 1488 1488
CONCEGUDA CONCEG
LEUYYYYRRAALAAA AHEEE CHARAALAAA AHEE CHARAALAAAA AHEE CHARAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
202 203 203 203 203 203 203 203 203 203
-3.652 -4.403 -3.688 -4.089 -4.811 -3.657 -4.066 -5.569 -3.355 -2.889 -3.291 -2.686 -1.707 -0.963 -0.773 -0.504 -0.117 0.155 0.339 -3.835 -4.435 -4.138 -5.246 -6.278 -7.524 -6.590 -7.661
31.212 31.813 31.337 31.337 31.337 30.574 30.577 31.923 32.177
1.995 2.1877 4.076 5.806 6.697 3.6527 3.6527 16.6379 16.6379 16.6379 17.216.429 19.19.19.19.19.19.19.19.19.19.19.19.19.1
1.00 26 1.00 26 1.00 26 1.00 26 1.00 26 1.00 26 1.00 3
9.25 2.01 3.15 2.76 3.22 2.03 3.69 1.68 6.06 8.14 9.74 2.79 4.56

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	15336 15337 15339 15442 15445 155445 15555 15556 1556667 155667 15667 15667	CE12 CCCCONCCCONCCCONCCCCCOCCONCCCCCCONCCCCCC	PHE PHE PHE GLU GLU GLU GLU GLU PRO PRO PRO PRO GLU	1008 1008 1008 1008 1009 1009 1009 1009	-8.346 -6.501 -7.535 -6.6676 -7.5429 -7.429 -7.5445 -5.0995 -8.1851 -8.995 -8.936 -7.821 -8.265 -9.1439 -7.738 -6.194 -4.121 -9.195 -10.426 -11.683	-9.165 -9.574 -10.756 -3.784 -3.2884 -1.5688 -1.5688 -1.7020 -0.9068 -1.4230 -0.9299 1.7028 4.0892 4.7745 4.6880 2.6886 4.77453 4.6886 5.0786 4.3876 4.3876 4.3876 4.3876 6.485 5.5996 6.485 6.4	29.305 27.806 27.806 26.946 27.5368 24.575 26.3887 24.5759 25.5306 24.5759 27.8558 27.8558 27.8558 27.8758 29.06819 30.5019 30	1.00 35.69 1.00 33.60 1.00 35.88 1.00 27.74 1.00 24.38 1.00 27.62 1.00 30.06 1.00 30.61 1.00 32.69 1.00 33.25 1.00 26.16 1.00 22.48 1.00 27.94 1.00 29.94 1.00 30.85 1.00 30.29 1.00 31.71 1.00 32.44 1.00 32.41 1.00 32.41 1.00 32.41 1.00 32.41 1.00 32.79 1.00 32.41 1.00 32.41 1.00 32.41 1.00 32.69 1.00 31.73 1.00 32.41 1.00 32.41 1.00 32.66 1.00 29.70 1.00 37.57 1.00 39.61 1.00 39.54 1.00 21.66 1.00 21.66 1.00 21.23 1.00 17.20	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1564 1565 1566 1567 1568 1569 1570	CD OE1 OE2 C O N CA	GLU GLU GLU GLY GLY	1012 1012 1012 1012 1012 1013 1013	-4.944 -4.121 -4.851 -9.195 -10.072 -9.457 -10.826	5.996 6.247 6.465 4.392 4.875 3.766 3.648	36.725 35.822 37.879 34.989 34.274 36.127 36.605 35.816 36.106 34.827 33.985 32.587 32.565	1.00 37.57 1.00 39.61 1.00 39.54 1.00 23.66 1.00 22.16 1.00 21.66 1.00 21.23	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1582 1583 1584 1585 1586 1587 1588 1589 1590	O N CB CG CE N C	GLY LYS LYS LYS LYS LYS LYS LYS LYS	1015 1016 1016 1016 1016 1016 1016 1016	-9.981 -9.231 -8.421 -7.608 -7.237 -6.578 -5.686 -4.279 -7.495 -7.530	-3.996 -2.275 -3.105 -2.244 -2.995 -2.101 -1.035 -1.489 -4.075 -5.270	35.711 34.488 33.623 32.648 31.354 30.302 30.921 31.073 34.326 34.045	1.00 21.89 1.00 21.98 1.00 22.53 1.00 23.14 1.00 23.43 1.00 22.86 1.00 18.96 1.00 21.09 1.00 22.81 1.00 25.20	

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MOTA	1592	N	THR	1017	-6.668	-3.583	35.233	1.00 23.2	
MOTA MOTA	1593 1594	CA CB	THR THR	1017 1017	-5.725 -4.878	-4.449	35.923 36.904	1.00 24.2 1.00 25.4	
ATOM	1595	OG1	THR	1017	-3.840	-3.638 -4.463	37.446	1.00 25.4 1.00 29.0	
ATOM	1596	CG2	THR	1017	-5.742	-3.107	38.027	1.00 29.8	33 B
ATOM ATOM	1597 1598	C	THR THR	1017 1017	-6.394 -5.852	-5.613 -6.719	36.658 36.708	1.00 25.1 1.00 25.2	17 B
ATOM	1599	O N	THR	1017	-7.580	-5.364	37.205	1.00 25.2	
MOTA	1600	CA	THR	1018	-8.328	-6.378	37.950	1.00 25.2	28 B
ATOM ATOM	1601 1602	CB OG1	THR THR	1018 1018	-9.414 -8.770	-5.701 -4.874	38.832 39.808	1.00 26.8	
ATOM	1603	CG2	THR	1018	-10.281	-6.737	39.550	1.00 23.	
ATOM	1604	C	THR	1018	-8.992	-7.404	37.039	1.00 24.2	21 B
ATOM ATOM	1605 1606	O N	THR VAL	1018 1019	-9.045 -9.486	-8.594 -6.931	37.359 35.902	1.00 22.9	
ATOM	1607	CA	VAL	1019	-10.164	-7.779	34.937	1.00 22.8	37 B
ATOM ATOM	1608 1609	CB CG1	VAL VAL	1019 1019	-10.888 -11.582	-6.932 -7.827	33.904 32.891	1.00 22.8 1.00 23.7	
ATOM	1610	CG2	VAL	1019	-11.872	-6.020	34.597	1.00 24.3	35 B
MOTA	1611	C	VAL	1019	-9.260	-8.755	34.187	1.00 24.3	10 B
MOTA MOTA	1612 1613	O N	$egin{array}{c} {\sf VAL} \\ {\sf ILE} \end{array}$	1019 1020	-9.572 -8.151	-9.944 -8.256	34.085 33.655	1.00 25.9 1.00 23.2	
MOTA	1614	CA	ILE	1020	-7.236	-9.101	32.900	1.00 24.4	48 B
ATOM ATOM	1615 1616	CB CG2	$_{\rm ILE}^{\rm ILE}$	1020 1020	-6.017 -5.168	-8.277 -7.764	32.367 33.515	1.00 23.7 1.00 22.0	
ATOM	1617	CG2	ILE	1020	-5.177	-9.129	31.411	1.00 22.0	91 B
ATOM	1618	CD1	ILE	1020	-3.957	-8.407	30.849	1.00 22.2	28 B
ATOM ATOM	1619 1620	C O	ILE ILE	1020 1020	-6.750 -6.756	-10.311 -11.436	33.698 33.190	1.00 25.0 1.00 24.0	
MOTA	1621	N	ASN	1021	-6.358	-10.090	34.950	1.00 27.3	37 B
ATOM ATOM	1622 1623	CA CB	ASN ASN	1021 1021	-5.868 -5.226	-11.169 -10.598	35.794 37.059	1.00 29.1 1.00 34.2	
ATOM	1624	CG	ASN	1021	-4.618	-10.598	37.039	1.00 39.8	31 B
ATOM	1625	OD1	ASN	1021	-4.761	-11.648	39.174	1.00 43.3	
ATOM ATOM	1626 1627	ND2 C	ASN ASN	1021 1021	-3.937 -6.942	-12.642 -12.190	37.327 36.166	1.00 39.9 1.00 28.9	
MOTA	1628	0	ASN	1021	-6.653	-13.382	36.230	1.00 30.7	74 B
ATOM ATOM	1629 1630	N CA	GLU GLU	1022 1022	-8.173 -9.276	-11.737 -12.646	36.410 36.767	1.00 29.4 1.00 28.7	
ATOM	1631	CB	GLU	1022	-10.574	-11.888	37.060	1.00 28.	74 B
ATOM	1632	CG	GLU	1022 1022	-10.505	-10.822	38.121	1.00 40.7	77 B
ATOM ATOM	1633 1634	CD OE1	GLU GLU	1022	-9.935 -9.841	-11.338 -12.578	39.407 39.561	1.00 44.9 1.00 47.0	
ATOM	1635	OE2	GLU	1022	-9.576	-10.498	40.262	1.00 49.3	32 B
ATOM ATOM	1636 1637	C 0	GLU GLU	1022 1022	-9.549 -9.694	-13.543 -14.759	35.583 35.713	1.00 26.3 1.00 23.6	
MOTA	1638	N	VAL	1023	-9.648	-12.901	34.425	1.00 23.8	36 B
ATOM	1639	CA	VAL	1023	-9.888	-13.582	33.171	1.00 22.2	
ATOM ATOM	1640 1641	CB CG1	VAL VAL	1023 1023	-9.934 -9.955	-12.570 -13.280	32.030 30.690	1.00 22.2 1.00 24.0	
MOTA	1642	CG2	VAL	1023	-11.140	-11.691	32.200	1.00 22.3	35 B
ATOM ATOM	1643 1644	C 0	VAL VAL	1023 1023	-8.750 -8.984	-14.568 -15.756	32.948 32.726	1.00 21.2 1.00 23.3	
MOTA	1645	N	TYR	1024	-7.523	-14.066	33.033	1.00 18.0	D3 В
ATOM ATOM	1646 1647	CA CB	TYR TYR	1024 1024	-6.335 -5.068	-14.880 -14.071	32.852 33.177	1.00 17.0 1.00 12.1	
ATOM	1648	CG	TYR	1024		-14.867	33.177	1.00 12.	

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ATOM 176 ATOM 176 ATOM 176 ATOM 176 ATOM 176 ATOM 176 ATOM 177 ATO
CD NE CZ NH1 CZ NH1 CZ NH2 CZ NH1 CZ NH2 CZ NH2 CZ NH2 CZ NH2 CZ CZ NH2 CZ CZ NH2 CZ CZ NZ CZ
ARG ARG GLU GLU GLU GLU GLU GLU GLU GLU GLU GRO PRO PRO PRO PRO PRO PRO PRO PRO PRO P
1037 1037 1037 1037 1037 1037 1037 1038 1038 1038 1038 1038 1038 1038 1039 1039 1039 1039 1039 1039 1040 1040 1041 1041 1041 1042 1042 1042
1.8814 1.0230 1.8814 1.0254 1.8823 1.0035 1.8814 1.0025 1.8814 1.0025 1.8823 1.0035 1.
-7.0992078 -7.099
33.1623 34.6634 36.6640 37.1298 39.1268 29.126.0025 20.1276.0025
1.00 30.81 1.00 32.69 1.00 35.51 1.00 34.79 1.00 34.18 1.00 25.92 1.00 25.92 1.00 26.43 1.00 29.29 1.00 33.57 1.00 34.71 1.00 31.34 1.00 27.23 1.00 27.23 1.00 24.99 1.00 25.96 1.00 25.96 1.00 25.96 1.00 25.96 1.00 25.96 1.00 26.84 1.00 16.70 1.00 16.87 1.00 16.70 1.00 16.70 1.00 16.87 1.00 16.87 1.00 16.64 1.00 16.70 1.00 16.64 1.00 25.43 1.00 22.22 1.00 22.22 1.00 22.32 1.00 25.55 1.00 25.43 1.00 25.43 1.00 25.43 1.00 25.43 1.00 25.55 1.00 26.61 1.00 25.43 1.00 27.96 1.00 26.84 1.00 27.96 1.00 27.96 1.00 26.84 1.00 27.96 1.00 27.96 1.00 27.96 1.00 28.65 1.00 27.96 1.00 28.65 1.00 27.96 1.00 28.65 1.00 27.96 1.00 28.65 1.00 27.96 1.00 27.96 1.00 28.65 1.00 27.96 1.00 27.96 1.00 28.65 1.00 29.23

Fig. 2A-31

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Fig. 2A-32

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Express Mall No.: EV 073687660 US

ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
18778901234567890012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678900123456789012345678901234567890123456789012345678900123456789000000000000000000000000000000000000
CCONCECCONCECONCEONCECONCECONCECONCECON
VAL VAL LEU LEU LEU LEU LEU LEU GLU GLU GLU GLU GLU GLU
$\begin{array}{c} 222222333333344444445555566666666667777788888888999999999999$
590287301636499456069874182899229395087350873448209 607296329739999356067323912339508735087350873508 607296329739999356067323995926735087348200 60729632973999935606772339951287357348200 607296329739999999999999999999999999999999
7.4176.7876.7876.7876.7876.7876.7876.7876.7
29.0188.205.139.14.0.98.50.15.86.66.81.38.33.33.33.33.33.33.33.33.33.33.33.33.
1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
34.35 32.30 28.97 29.72 30.37 32.29

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
1934 1935 1937 1937 1937 1937 1937 1937 1937 1937
N C B C C C C C C C C C C C C C C C C C
ILE
1060 1060 1060 1060 1060 1060 1060 1060
8.364 5.869 5.5816 5.5816 7.5073 8.59920 7.5073 8.59920 7.5073 8.59920 7.5073 8.59920 7.5073 8.59920 7.5073 7.5
14.815 13.725 14.667 15.307 15.713 11.824 11.924 11.926 12.926 12.926 12.926 12.926 12.926 13.926 13.926 13.926 13.926 13.926 14.926 14.926 15.926 16.836 17.636 18.927 19.926 19
24.6130 24.6730 24.6730 24.6730 26.7455 23.7652 23.3124 24.7653 23.322 23.3124 24.319 24.319 25.319 26.319 27.319 28.319
1.00 25.40 1.00 23.86 1.00 24.13 1.00 26.24 1.00 25.30 1.00 24.57 1.00 22.61 1.00 23.44 1.00 20.99 1.00 20.45 1.00 21.03 1.00 23.60 1.00 23.60 1.00 19.01 1.00 18.92 1.00 18.92 1.00 19.68 1.00 19.11 1.00 18.81 1.00 16.28 1.00 21.57 1.00 21.57 1.00 22.15 1.00 24.67 1.00 33.22 1.00 37.24 1.00 37.20 1.00 38.73 1.00 17.42 1.00 15.48 1.00 16.19 1.00 18.81 1.00 16.46 1.00 13.15 1.00 18.81 1.00 16.46 1.00 13.15 1.00 18.41 1.00 16.46 1.00 13.15 1.00 18.41 1.00 16.46 1.00 13.15 1.00 18.41 1.00 18.27 1.00 18.41 1.00 19.49 1.00 16.46 1.00 13.15 1.00 18.31 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.49 1.00 19.501

Fig. 2A-34

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
199344567899012345678990112345678901223456789012232222222222222222222222222222222222
CCCCCCCCONCCCONCCCONCCCCNCNNCONCCCNCNNCONCCCCCC
PHE PHE PHE PHE ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
106771067710667710667710667710667710667710667710667710667710667710667710668888899999900070071107110711077110771107
8.8531 6.8531 76.15106 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2045 77.2056
3.369175 4.696175 4.696175 4.696175 4.69670307 5.31696175 4.69670307 5.316972
24.8364 24.8364 24.8364 27.3129 28.673129 28.67332 29.273.4733 20.866724 20.866724 20.866724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86733 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.86724 20.8736 20.87
1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
23.54 26.00 29.26 28.46 31.80 31.72 22.70 24.34 19.20 16.13 14.28 13.59 14.90 14.47 14.87 14.87 15.57 15.28 16.49 19.93

Fig. 2A-35

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
22222222222222222222222222222222222222
ND1 CE1 CONCACCCCCONCACCCCCCCCCCCCCCCCCCCCCCCCC
VAL VAL LEU LEU LEU LEU LEU LYS LYS LYS LYS LYS LYS LYS LYS LYS
$\begin{array}{c} 107444444441\\ 1077444444555555555555666666777777777788888889999999999$
5.208 4.439 3.118 4.170 5.322 4.716 6.105 6.249 7.196 7.556 6.492 6.983 6.678
-6.972 -6.133 -6.918 -7.155 -7.596 -8.217 -7.966 -7.774 -8.824 -7.286 -7.975 -6.993 -7.174 -6.033 -9.117 -10.285 -8.767 -9.714 -8.940 -8.082 -8.048 -10.375 -11.850 -11.857 -9.765 -12.025 -11.658 -12.310 -11.702 -12.951 -11.658 -12.310 -11.702 -12.951 -11.528 -12.734 -13.881 -11.702 -12.048 -12.734 -13.881 -11.528 -12.551 -13.551 -12.586 -13.511
23.342 24.946 25.5775 26.7756 27.066 27.066 27.066 27.066 27.066 27.066 27.066 27.066 27.0766
1.00 16.1 1.00 16.1 1.00 13.8 1.00 10.3 1.00 10.0 1.00 17.9 1.00 18.2 1.00 19.1 1.00 18.5 1.00 18.5 1.00 14.9 1.00 22.6 1.00 23.3 1.00 23.3 1.00 24.3 1.00 23.3 1.00 23.3 1.00 21.4 1.00 23.3 1.00 21.4 1.00 23.3 1.00 21.4 1.00 23.3 1.00 21.4 1.00 16.1 1.00 17.1 1.00 17.1 1.00 16.1 1.00 17.1 1.00 16.1 1.00 17.1 1.00 16.1 1.00 16.1 1.00 17.1 1.00 16.1 1.00 16.1 1.00 17.1 1.00 16.1
3532292021041476854624085823551599137165906409142075324

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2105 2106 2107 2108 2109 2110 2111 2112 2113 2114 2115 2116 2117 2118 2119 2120 2121 2122 2123 2124 2125 2126 2127 2128 2130 2131 2132 2133 2134 2135 2136	N CD CB CG CD CC CD CC CD CC CD CC CC CC CC CC CC	PRO PRO PRO PRO PRO PRO ALA ALA ALA ALA LEU LEU LEU LEU LEU LYS	1081 1081 1081 1081 1081 1082 1082 1082	7.763 -15.008	B B B B B B B B B B B B B B B B B B B
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2139 2140 2141 2142 2143 2144 2145 2146 2147 2148 2150 2151 2152 2153 2154 2155 2156 2157 2158 2160 2161	OE1 OE2 C O N CA C O N CA CB CC N CA CB CC	GLU GLU GLU GLY GLY GLY GLY LYS LYS LYS LYS LYS LYS LYS LYS LYS L	1085 1085 1085 1086 1086 1086 1087 1087 1087 1087 1087 1088 1088 1088	6.608 -23.540	888888888888888888888888888888888888888

Fig. 2A-37

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2162 2163 2164 2165 2166 2167 2168 2170 2171 2172 2173 2174 2175 2176 2177 2180 2181 2182 2183 2184 2185 2188 2189 2190 2191 2193	O N CA CB CG1 CC CO N CA CB CCD1 CCD2 C O N CA CB CCD1 CCD2 C O N CA CCB CCC CC CCC CCC CCC CCC CCC CCC C	VAL VAL VAL VAL VAL LEU LEU LEU LEU LEU CYS CYS CYS CYS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	1088 1089 1089 1089 1089 1089 1089 1090 1090	-1.697 -1.090	-14.210 -13.777 -13.315 -12.676 -12.970 -12.233 -12.753 -11.596 -13.213 -13.519 -12.990 -10.478 -10.688 -9.307 -8.156 -7.734 -6.757 -7.013 -6.782 -6.293 -5.205 -4.840 -5.155 -4.853 -5.712 -3.946 -3.508 -3.341	25.182 23.793 24.797 24.355 22.931 25.254 25.094 24.185 26.376 26.797 27.993 27.915 29.299 26.965 27.182 26.837 25.547 25.782 27.356 26.837 25.782 27.356 26.833 28.378 28.887 30.661 29.835 31.760 28.044 27.551 27.880 27.093	1.00 16.14 1.00 19.93 1.00 20.79 1.00 23.46 1.00 21.64 1.00 19.98 1.00 20.42 1.00 18.26 1.00 18.09 1.00 16.30 1.00 16.30 1.00 16.30 1.00 16.59 1.00 16.59 1.00 16.59 1.00 16.59 1.00 20.36	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2195 2196 2197 2198 2199 2200 2201 2202 2203 2204 2205 2206	CB CG CD NE CZ NH1 NH2 C O N CA CB CG	ARG ARG ARG ARG ARG ARG ARG TYR TYR TYR	1093 1093 1093 1093 1093 1093 1093 1094 1094 1094	-0.364 -1.079 -0.116 -0.013 0.070 0.064 0.163 -0.710 0.161 -1.232 -0.749 -1.493 -0.635	-0.336 0.489 -0.025 0.731 2.059 0.156 -2.384 -3.233 -1.676 -1.842 -2.967 -3.606	27.826 28.937 29.801 31.175 32.271 32.186 33.463 25.688 25.509 24.690 23.327 22.595 21.522	1.00 33.34 1.00 41.29 1.00 53.87 1.00 56.53 1.00 57.47 1.00 57.04 1.00 27.93 1.00 26.93 1.00 25.26 1.00 23.35 1.00 24.45 1.00 23.14	E E E E E E E E E E E E E E E E E E E
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2207 2208 2209 2210 2211 2212 2213 2214 2215 2216 2217 2218	CD1 CE1 CD2 CE2 CZ OH C O N CA CB	TYR TYR TYR TYR TYR TYR TYR ILE ILE ILE	1094 1094 1094 1094 1094 1094 1095 1095 1095	0.662 1.504 -1.086 -0.252 1.042 1.895 -0.843 -0.866 -0.899 -0.952 -0.908	-4.029 -4.534 -3.723 -4.230 -4.632 -5.106 -0.551 0.524 -0.665 0.496 0.069	21.815 20.822 20.202 19.197 19.518 18.543 22.526 23.106 21.198 20.310 18.803 18.542	1.00 22.25 1.00 22.52 1.00 21.33 1.00 23.16 1.00 19.75 1.00 22.64 1.00 22.73 1.00 23.36 1.00 22.04 1.00 20.47	E E E E E E E E E E E E E E E E E E E

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ATOM 2: ATOM 3: ATOM 3
219 CG1 2210 CD1 2211 C O 2223 N CA 2224 CA 2225 CD1 2229 C OD1 2229 C OD2 2230 C CA 2231 CA 2232 C CB 2237 CA 2332 CB 2334 CC 2337 CA 2338 CB 2337 CA 2338 CB 2440 CC 2441 CD 2442 CD 2443 CC 2443 CC 2443 CC 2443 CC 2443 CC 255 CC 256 CC 257 CC 258 CC 257
LLE LPPPPPRRRRRRRRRRRRUUUUUUUAAALAATTYYYYRRRRRRNNNNNN
1095 1095 1095 1096 1096 1096 1096 1097 1097 1097 1097 1097 10997 1099 1099
$\begin{array}{c} -2.166 \\ -2.1920 \\ -2.1920 \\ -3.3477 \\ -5.85790 \\ -4.7579 \\ -6.1260 \\ -6.1260 \\ -2.1920 \\ -3.3779 \\ -2.1920 \\ -3.3779 \\ -2.1920 \\$
-0.46822 -1.46822 -1.46822 -1.46864 -1.4683460 -1.4683460 -1.1053465 -1.201.105346 -1.
18.419 17.034 20.523 20.814 21.229 21.20.801 21.229 21.220.221 22.220.2201 22.2
1.00 24.32 1.00 22.17 1.00 25.34 1.00 26.58 1.00 26.18 1.00 29.67 1.00 32.52 1.00 37.98 1.00 23.76 1.00 24.70 1.00 23.24 1.00 21.75 1.00 20.27 1.00 20.27 1.00 19.17 1.00 19.17 1.00 19.17 1.00 19.23 1.00 23.68 1.00 23.68 1.00 23.68 1.00 23.68 1.00 23.68 1.00 24.34 1.00 23.68 1.00 24.34 1.00 23.63 1.00 24.34 1.00 25.84 1.00 24.50 1.00 25.84 1.00 24.50 1.00 25.84 1.00 24.50 1.00 25.84 1.00 27.16 1.00 28.25 1.00 27.16 1.00 27.16 1.00 28.25 1.00 27.16 1.00 27.16 1.00 27.16 1.00 27.16 1.00 27.16 1.00 28.25 1.00 27.16 1.00 2
888888888888888888888888888888888888

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ATOM 22: ATOM 23: ATO
77
TYR TYR TYR TYR ALA ALA ARG ARG ARG ARG ARG ARG ARG ARG ARG AR
1102 1103 1103 1103 1104 1104 1104 1104 1104
0.028 -1.435 -2.6389 -2.9289 -4.4639 -7.00992 -7.899342 -7.899342 -7.89.3388 -4.6663 -4.5245 -1.5661663 -4.721 -1.5661663 -4.721 -1.720 -1.752
11.996 10.111 10.542 11.447 12.096 11.476 11.4575 12.279977 13.69885 14.312.193 14.9087 13.193 14.9087 14.46021 14.9087 14.4593 14.4593 14.5531 14.5531 15.3850 14.5393 15.3850 14.5393 15.3850 14.5949 15.3850 14.5949 16.4851 17.5949 17.663 1
21.916 20.168 19.187 21.5547 21.55547 21.55547 22.7720.639 22.7732 22.
1.00 32.4 1.00 39.6 1.00 29.6 1.00 29.6 1.00 30.3 1.00 29.2 1.00 31.8 1.00 32.5 1.00 32.7 1.00 33.1 1.00 32.1 1.00 32.1 1.00 32.1 1.00 32.1 1.00 26.9 1.00 27.6 1.00 27.6 1.00 25.3 1.00 25.3 1.00 25.3 1.00 25.3 1.00 25.3 1.00 25.3 1.00 25.3 1.00 27.6 1.00 27.6
27 8 <t< td=""></t<>

Fig. 2A-40

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
22222222222222222222222222222222222222
CABGD12 CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
ARG ARG ALA ALA ALA ALA LEU LEU LEU LEU LEU LEU ASN ASN ASN ASN
1111 1111 1111 1111 1111 1111 1111 1111 1111
0.6 0.8 1.8 2.8 0.8 1.8 0.8 1.8 1.8 1.8 1.8 1.8 1.8 1.8 1.8 1.8 1
633422900089750043486452114715773447599466073688772740
10.08899179600445253462666007166283996589844120043626602377545556557733332223334101.
12.3973 12.3971023 12.3971023 12.3971023 12.3971023 12.3971023 12.306124 13.30728861 14.308873 12.308861 14.308861 15.308861 16.308
1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
40.15 44.62 45.80 43.93 27.92 26.58 27.44 26.88 30.38 34.98 34.07 43.10 24.78 22.58 21.00 21.29 22.71 27.34 29.25 33.08 42.60 41.67 45.60 23.40 23.40 23.69 21.65

Fig. 2A-41

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ATOM 2391 CB GLU 1 ATOM 2392 CG GLU 1 ATOM 2393 CD GLU 1 ATOM 2394 OE1 GLU 1 ATOM 2395 OE2 GLU 1 ATOM 2396 C GLU 1 ATOM 2397 O GLU 1 ATOM 2398 N PHE 1 ATOM 2399 CA PHE 1 ATOM 2400 CB PHE 1 ATOM 2401 CG PHE 1 ATOM 2401 CG PHE 1 ATOM 2403 CD2 PHE 1 ATOM 2404 CE1 PHE 1 ATOM 2405 CE2 PHE 1 ATOM 2406 CZ PHE 1 ATOM 2407 C PHE 1 ATOM 2408 O PHE 1 ATOM 2409 N ALA 1 ATOM 2410 CA ALA 1 ATOM 2411 CB ALA 1 ATOM 2411 CB ALA 1 ATOM 2412 C ALA 1 ATOM 2412 C ALA 1 ATOM 2413 O ALA 1 ATOM 2414 N ILE 1 ATOM 2415 CA ILE 1 ATOM 2416 CB ILE 1 ATOM 2417 CG2 ILE 1 ATOM 2418 CG1 ILE 1 ATOM 2419 CD1 ILE 1 ATOM 2410 CA ASN 1 ATOM 2411 CB ASN 1 ATOM 2412 C ALA 1 ATOM 2412 C ALA 1 ATOM 2413 CA ASN 1 ATOM 2414 CB ASN 1 ATOM 2415 CA ILE 1 ATOM 2416 CB ILE 1 ATOM 2417 CG2 ILE 1 ATOM 2421 C ILE 1 ATOM 2420 C ILE 1 ATOM 2421 CA ASN 1 ATOM 2422 CA ASN 1 ATOM 2423 CA ASN 1 ATOM 2424 CB ASN 1 ATOM 2423 CA ASN 1 ATOM 2424 CB ASN 1 ATOM 2424 CB ASN 1 ATOM 2425 CG ASN 1 ATOM 2426 OD1 ASN 1 ATOM 2427 ND2 ASN 1 ATOM 2428 C ASN 1 ATOM 2429 C ASN 1 ATOM 2421 CA GLY 1 ATOM 2433 CA SN 1 ATOM 2434 N LEU 1 ATOM 2434 N LEU 1 ATOM 2435 CA LEU 1 ATOM 2436 CB LEU 1 ATOM 2437 CG LEU 1 ATOM 2438 CD1 LEU 1 ATOM 2438 CD1 LEU 1 ATOM 2438 CD1 LEU 1 ATOM 2439 CD2 LEU 1 ATOM 2439 CD2 LEU 1 ATOM 2439 CD2 LEU 1 ATOM 2430 N CD2 LEU 1 ATOM 2431 CA TYR 1
1123 0.440 1124 2.268 1124 1.661 1124 2.707 1124 2.360
0.705 12.703 1.350 11.418 1.619 11.426 2.624 10.364 3.207 9.705 2.831 10.189 0.286 12.490 -0.828 12.051 1.191 12.797 0.921 12.633 2.235 12.687 2.101 12.269 2.043 10.917 2.013 13.223 1.895 10.522 1.864 12.835 1.805 11.478 -0.023 13.739 -0.892 13.519 0.157 14.922 -0.651 16.099 0.030 17.376 -2.056 16.025 -3.010 16.375 -2.171 15.570 -3.462 17.194 -2.746 14.828 -2.568 15.225 -4.143 14.133 -5.266 -3.470 13.148 -2.568 15.225 -4.143 14.133 -5.266 -3.470 13.148 -2.568 15.225 -4.143 14.133 -5.266 -3.470 13.148 -2.568 15.225 -4.143 14.133 -5.266 13.986 -3.470 13.148 -4.035 11.807 -4.768 11.698 -5.078 10.092 -4.990 11.381 -6.062 10.092 -4.990 11.381 -6.151 11.071 -4.509 11.383 -5.343 10.965 -6.990 14.830 -7.731 15.196 -8.859 14.830 -7.7731 15.196 -8.859 14.830 -9.238 16.945 -6.599 14.830 -5.765 15.697 -6.903 14.404 -6.316 15.010 -5.823 13.964
1.00 21.22 1.00 22.82 1.00 29.23 1.00 34.01 1.00 37.19 1.00 17.40 1.00 16.29 1.00 16.74 1.00 15.46 1.00 17.12 1.00 17.63 1.00 16.85 1.00 16.85 1.00 16.85 1.00 16.85 1.00 15.09 1.00 15.09 1.00 15.09 1.00 17.65 1.00 21.11 1.00 20.85 1.00 21.11 1.00 21.11 1.00 21.11 1.00 21.11 1.00 21.69 1.00 21.69 1.00 21.69 1.00 21.69 1.00 21.69 1.00 23.81 1.00 24.30 1.00 25.43 1.00 27.35 1.00 23.66 1.00 23.66 1.00 21.50 1.00 23.68 1.00 23.68 1.00 23.68 1.00 21.14 1.00 20.80 1.00 21.14
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ATOM 244 ATOM 245 ATOM 245 ATOM 245 ATOM 245 ATOM 245 ATOM 245 ATOM 246 ATOM 246 ATOM 246 ATOM 246 ATOM 246 ATOM 246 ATOM 247 ATOM 248 ATO
CD2 CD2 CC2 CO OH CC3 CC4 CC5 CC5 CC5 CC6 CC6 CC7 CC6 CC7 CC7 CC7 CC7 CC7 CC7
TYR TYR TYR PRO PRO PRO PRO PRO PRO ASP ASP ASP ASP ASP ASP LEU LEU LHR THR THR THR THR THR THR THR THR THR
1125 1125 1125 1125 1125 1126 1126 1126
-4.513 -3.897 -7.662 -8.730 -7.581 -8.762
$\begin{array}{c} -3.4411\\ -3.16150\\ -2.08260\\ -1.21826$
11.49588 11.49888 11.6197 12.3.4163 13.416.8197 13.416.8197 15.848089 16.379586 17.7.898289 17.7.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 17.89828 18.
1.00 24.88 1.00 23.01 1.00 24.99 1.00 25.15 1.00 28.59 1.00 22.66 1.00 21.46 1.00 22.02 1.00 22.11 1.00 22.45 1.00 21.26 1.00 21.43 1.00 20.33 1.00 20.02 1.00 19.31 1.00 20.62 1.00 21.79 1.00 23.88 1.00 20.62 1.00 17.79 1.00 18.84 1.00 16.50 1.00 17.71 1.00 16.50 1.00 17.61 1.00 16.59 1.00 17.61 1.00 16.39 1.00 16.39 1.00 17.61 1.00 16.39 1.00 16.39 1.00 17.61 1.00 16.39 1.00 17.61 1.00 16.39 1.00 17.61 1.00 16.39 1.00 17.61 1.00 16.39 1.00 17.61 1.00 16.59 1.00 17.61 1.00 16.39 1.00 17.61 1.00 17.61

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Fig. 2A-44

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ATOM	2561	CC	NDC	1140	-13.556	11.340	39.202	1.00 22.94	ח
ATOM	2562	CG CD	ARG ARG	1140 1140	-14.684	12.235	39.739	1.00 22.94 1.00 20.22	B B
ATOM	2563	NE	ARG	1140	-15.681	12.546	38.723	1.00 20.22	В
ATOM	2564	CZ	ARG	1140	-16.985	12.340	38.873	1.00 17.31	В
ATOM	2565	NH1	ARG	1140	-17.464	11.859	40.004	1.00 17.85	В
ATOM	2566	NH2		1140	-17.813	12.686	37.891	1.00 16.17	В
ATOM	2567	C	ARG	1140	-13.517	8.307	39.777	1.00 23.64	В
ATOM	2568	ŏ	ARG	1140	-12.574	8.289	40.586	1.00 22.06	В
ATOM	2569	Ň	GLU	1141	-14.717	7.812	40.068	1.00 24.14	B
MOTA	2570	CA	GLU	1141	-15.024	7.242	41.374	1.00 24.75	В
MOTA	2571	CB	GLU	1141	-16.515	6.969	41.470	1.00 22.97	В
MOTA	2572	CG	GLU	1141	-17.347	8.221	41.315	1.00 27.60	В
MOTA	2573	CD	GLU	1141	-17.062	9.248	42.401	1.00 30.88	В
MOTA	2574	OE1	GLU	1141	-16.549	8.855	43.473	1.00 33.55	В
ATOM	2575	OE2	GLU	1141	-17.347	10.448	42.193	1.00 31.14	В
ATOM	2576	C	GLU	1141	-14.253	5.981	41.708	1.00 25.69	В
MOTA	2577 2578	0	GLU	$\frac{1141}{1142}$	-13.948 -13.939	5.730	42.873 40.698	1.00 28.51 1.00 25.82	В
ATOM ATOM	2579	N	ARG ARG	1142	-13.192	5.182 3.952	40.696	1.00 25.82 1.00 26.19	B B
ATOM	2580	CA CB	ARG	1142	-13.144	3.122	39.638	1.00 26.22	В
ATOM	2581	CG	ARG	1142	-13.794	1.755	39.795	1.00 25.35	В
MOTA	2582	CD	ARG	1142	-13.757	0.924	38.527	1.00 21.26	B
MOTA	2583	NE	ARG	1142	-15.010	0.197	38.377	1.00 18.77	В
MOTA	2584	CZ	ARG	1142	-15.589	-0.051	37.210	1.00 18.03	В
MOTA	2585	NH1		1142	-16.734	-0.717	37.166	1.00 16.76	В
MOTA	2586	NH2		1142	-15.015	0.361	36.089	1.00 18.02	В
ATOM	2587	C	ARG	1142	-11.776	4.242	41.428	1.00 26.05	В
MOTA	2588	0	ARG	1142	-11.274	3.543	42.311	1.00 26.26	В
ATOM ATOM	2589 2590	N CA	$_{\rm ILE}^{\rm ILE}$	1143 1143	-11.149 -9.796	5.278 5.692	40.867 41.248	1.00 25.61 1.00 26.53	B B
ATOM	2591	CB	ILE	1143	-9.282	6.804	40.322	1.00 24.83	В
ATOM	2592	CG2	ILE	1143	-8.182	7.584	41.013	1.00 24.32	В
ATOM	2593	CG1	ILE	1143	-8.783	6.200	39.006	1.00 24.83	B
MOTA	2594	CD1	ILE	1143	-9.255	6.944	37.758	1.00 20.76	В
MOTA	2595	С	ILE	1143	-9.766	6.232	42.684	1.00 28.39	В
MOTA	2596	0	ILE	1143	-8.823	5.989	43.440	1.00 28.02	В
MOTA	2597	N	ILE	1144	-10.800	6.983	43.040	1.00 29.81	В
ATOM	2598	CA	ILE	1144	-10.913	7.556	44.372	1.00 31.98	В
ATOM	2599	CB	ILE	1144	-11.593	8.948	44.299	1.00 33.00	В
ATOM ATOM	2600 2601	CG2	ILE	1144	-13.086 -10.970	8.821 9.889	44.546	1.00 34.57 1.00 34.56	B B
ATOM	2602	CG1 CD1	ILE ILE	$\frac{1144}{1144}$	-9.885	10.798	45.326 44.760	1.00 34.30	В
ATOM	2603		ILE	1144		6.628		1.00 30.20	В
ATOM	2604	ŏ	ILE	1144	-11.327	5.482	45.551	1.00 32.67	B
MOTA	2605	Ň	GLN	1155	-8.229	18.229	42.196	1.00 60.55	В
MOTA	2606	CA	GLN	1155	-7.582	17.663	41.021	1.00 60.30	В
MOTA	2607	CB	GLN	1155	-8.084	16.233	40.768	1.00 63.31	В
ATOM	2608	CG	GLN	1155	-8.108	15.325	42.008	1.00 69.16	В
MOTA	2609	CD	GLN	1155	-6.713	14.929	42.502	1.00 73.40	В
MOTA	2610	OE1	GLN	1155	-6.573	14.133	43.443	1.00 74.63	В
MOTA MOTA	2611 2612	NE2 C	GLN GLN	1155 1155	-5.677 - 7.835	15.484 18.520	41.870 39.784	1.00 75.02 1.00 58.58	B B
ATOM	2613	0	GLN	1155	-6.895	19.052	39.784	1.00 58.70	В
MOTA	2614	N	GLU	1156	-9.107	18.658	39.408	1.00 56.35	В
ATOM	2615	CA	GLU	1156	-9.493	19.431	38.225	1.00 54.17	В
MOTA	2616	CB	GLU	1156	-9.286	20.929	38.460	1.00 54.85	В
MOTA	2617	CG	GLU	1156	-10.533	21.648	38.936	1.00 54.77	В

Fig. 2A-45

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM
8901234567890123456789012345678901234 61622222222222222222222222222222222222
CD GLU OE1 GLU OE2 GLU OE2 GLU OE2 GLU OE2 GLU OE2 GLU OE3 GLU OE3 GLU OE3 GLU OE4 ASP CB ASP CB ASP CCB ASP CCB LEU CCB LEU CCB LEU CCB CCC C
1156 1156 1156 1157 1157 1157 1157 1157
-11.199 -10.720 -8.6083 -7.9249 -8.6083 -7.11.86693 -7.11.970 -8.6083 -7.11.970 -8.6083 -7.11.970 -10.12.74.00 -11.5740 -11.5740 -11.74.00 -11.74.00 -11.74.00 -11.75.00 -11.76.
21.033 21.441 20.0566 19.597 17.8205 11.6.357 17.8205 11.5.223 13.377 12.3579 12.3579 14.456 15.4912 15.642 15.643 16.243 16.243 16.257 16.257 16.257 16.257 16.257 16.257 16.257 16.257 16.260 17.207 16.257
40.1291 41.2924 41.2924 41.2924 41.2924 41.2924 41.2924 41.2924 41.2924 41.2924 41.2924 41.2924 42.2925 42.2925 43.
1.00 55.73 1.00 56.94 1.00 56.37 1.00 52.69 1.00 51.58 1.00 51.79 1.00 49.12 1.00 49.00 1.00 49.78 1.00 50.10 1.00 46.67 1.00 45.76 1.00 43.63 1.00 41.40 1.00 41.39 1.00 40.74 1.00 41.01 1.00 38.87 1.00 40.29 1.00 40.06 1.00 39.05 1.00 39.66 1.00 41.01 1.00 41.48 1.00 41.35 1.00 37.36

Fig. 2A-46

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ATOM	2675	OE2	GLU	1162	-16.052	14.954	30.186	1.00 50.60	В
ATOM	2676	CEZ	GLU	1162	-11.161	12.908	28.590	1.00 33.86	В
ATOM	2677	ŏ	GLU	1162	-11.866	12.649	27.614	1.00 32.85	B
ATOM	2678	N	LYS	1163	-9.881	13.260	28.481	1.00 31.94	В
MOTA	2679	CA	LYS	1163	-9.222	13.364	27.176	1.00 31.73	В
MOTA	2680	CB	LYS	1163	-7.893	14.115	27.282	1.00 32.90	В
MOTA	2681	CG	LYS	1163	-7.950	15.612	27.073	1.00 34.32	В
ATOM	2682	CD	LYS	1163	-6.901	16.253	27.969	1.00 38.71	В
ATOM	2683 2684	CE	LYS LYS	1163 1163	-7.052 -5.774	17.760 18.375	28.089 28.577	1.00 39.61 1.00 39.38	В В
MOTA MOTA	2685	NZ C	LYS	1163	-8.935	11.991	26.585	1.00 39.38	В
ATOM	2686	Ö	LYS	1163	-9.203	11.746	25.411	1.00 30.23	В
ATOM	2687	Ň	VAL	1164	-8.365	11.106	27.397	1.00 27.87	В
ATOM	2688	CA	VAL	1164	-8.038	9.762	26.946	1.00 27.20	В
ATOM	2689	CB	VAL	1164	-7.331	8.968	28.054	1.00 26.82	В
MOTA	2690	CG1	VAL	1164	-6.748	7.686	27.472	1.00 28.40 1.00 24.86	B B
ATOM ATOM	2691 2692	CG2 C	VAL VAL	1164 1164	-6.230 -9.296	9.826 9.021	28.684 26.513	1.00 24.88	В
ATOM	2693	Õ	VAL	1164	-9.333	8.439	25.432	1.00 26.76	В
ATOM	2694	Ň	ILE	1165	-10.332	9.064	27.354	1.00 31.31	B
MOTA	2695	CA	ILE	1165	-11.603	8.399	27.058	1.00 31.66	В
MOTA	2696	CB	ILE	1165	-12.667	8.687	28.145	1.00 32.11	В
ATOM	2697	CG2	ILE	1165	-14.013	8.082	27.733	1.00 30.75	В
MOTA MOTA	2698 2699	CG1 CD1	ILE ILE	1165 1165	-12.220 -13.181	8.098 8.374	29.486 30.633	1.00 31.53 1.00 31.11	B B
ATOM	2700	CDI	ILE	1165	-12.174	8.820	25.706	1.00 31.11	В
ATOM	2701	ŏ	ILE	1165	-12.857	8.036	25.051	1.00 34.16	B
MOTA	2702	N	GLU	1166	-11.922	10.059	25.297	1.00 34.96	В
MOTA	2703	CA	GLU	1166	-12.418	10.512	24.005	1.00 35.90	В
ATOM	2704	CB	GLU	1166	-12.439	12.042	23.911	1.00 40.19	В
ATOM ATOM	2705 2706	CG CD	GLU GLU	1166 1166	-13.254 -13.408	12.540 14.054	22.718 22.670	1.00 48.35 1.00 53.25	B B
ATOM	2707	OE1	GLU	1166	-13.548	14.678	23.746	1.00 56.10	В
ATOM	2708	OE2	GLÜ	1166	-13.395	14.621	21.553	1.00 54.50	В
MOTA	2709	С	GLU	1166	-11.528	9.936	22.908	1.00 34.58	В
MOTA	2710	0	GLU	1166	-11.974	9.748	21.777	1.00 35.86	В
ATOM	2711	N	GLY	1167	-10.270	9.654	23.248	1.00 33.49	В
ATOM ATOM	2712 2713	CA C	GLY GLY	1167 1167	-9.347 - 9.755	9.076 7.646	22.279 21.953	1.00 29.33 1.00 28.37	B B
ATOM	2713	Ö	GLY	1167	-9.763	7.225	20.787	1.00 27.68	В
ATOM	2715	Ň	TYR	1168	-10.115	6.905	22.999	1.00 26.42	В
MOTA	2716	CA	TYR	1168	-10.549	5.522	22.878	1.00 23.05	В
MOTA	2717	CB	TYR	1168	-10.635	4.886	24.266	1.00 19.40	В
MOTA	2718	CG CD1	TYR	1168	-9.325	4.333	24.804	1.00 17.64 1.00 15.43	В
ATOM ATOM	2719 2720	CD1 CE1	TYR TYR	1168 1168	-8.857 -7.686	4.689 4.132	26.070 26.590	1.00 15.43 1.00 12.34	B B
ATOM	2721	CD2	TYR	1168	-8.576	3.410	24.067	1.00 12.34	В
ATOM	2722	CE2	TYR	1168	-7.396	2.848	24.587	1.00 15.67	В
MOTA	2723	CZ	TYR	1168	-6.965	3.212	25.847	1.00 11.37	В
ATOM	2724	OH	TYR	1168	-5.836	2.624	26.369	1.00 11.10	В
ATOM	2725 2726	С	TYR	1168 1168	-11.916	5.465	22.200 21.317	1.00 24.16 1.00 25.88	В В
MOTA MOTA	2727	O N	TYR GLN	1168	-12.147 -12.819	4.637 6.352	22.617	1.00 25.88	В
ATOM	2728	CA	GLN	1169	-14.169	6.409	22.056	1.00 25.80	В
MOTA	2729	CB	GLN	1169	-15.003	7.482	22.769	1.00 28.84	В
ATOM	2730	CG	GLN	1169	-15.561	7.074	24.138	1.00 32.63	В
ATOM	2731	CD	GLN	1169	-16.011	5.622	24.190	1.00 33.87	В

Fig. 2A-47

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A III OM	2222	ΩΠ1	CTN	1160	15 500	4 040	05 051	1 00 25 00	. 5
ATOM ATOM	2732 2733	OE1 NE2		1169 1169	-15.583 -16.876	4.849 5.244	25.051 23.262	1.00 35.90 1.00 38.23	B B
ATOM	2734	C	GLN	1169	-14.118	6.723	20.572	1.00 25.68	В
MOTA	2735	0	GLN	1169	-13.233	7.452	20.114	1.00 27.45	В
ATOM	2736	N	PHE	1179	-12.329	-5.199	17.978	1.00 31.48	В
MOTA	2737	CA	PHE	1179	-12.665	-4.453	19.207	1.00 33.93	В
ATOM ATOM	2738 2739	CB CG	PHE PHE	1179 1179	-12.948 -11.709	-2.982 -2.184	18.891 18.648	1.00 32.21 1.00 32.23	В
ATOM	2740	CD1		1179	-11.709	-2.164 -1.953	17.354	1.00 32.23	B B
ATOM	2741	CD2	PHE	1179	-10.941	-1.733	19.720	1.00 31.20	В
MOTA	2742	CE1	PHE	1179	-10.076	-1.291	17.129	1.00 32.53	В
MOTA	2743	CE2		1179	-9.749	-1.070	19.505	1.00 29.40	В
ATOM ATOM	2744 2745	CZ	PHE PHE	1179 1179	-9.312 -13.860	-0.849	18.213	1.00 32.25	В
ATOM	2745	C O	PHE	1179	-13.860 -14.970	-5.029 -5.073	19.939 19.415	1.00 33.62 1.00 37.56	B B
ATOM	2747	N	LYS	1180	-13.636	-5.463	21.163	1.00 37.30	В
ATOM	2748	CA	LYS	1180	-14.724	-6.001	21.936	1.00 32.44	B
MOTA	2749	CB	LYS	1180	-14.402	-7.386	22.472	1.00 32.29	В
ATOM	2750	CG	LYS	1180	-14.173	-8.419	21.395	1.00 32.85	В
ATOM ATOM	2751 2752	CD CE	LYS LYS	1180 1180	-15.306 -15.377	-8.408 -9.731	20.400 19.653	1.00 34.11 1.00 38.27	B B
ATOM	2753	NZ	LYS	1180	-16.742	-10.036	19.117	1.00 38.28	В
ATOM	2754	C	LYS	1180	-14.897	-5.041	23.063	1.00 32.57	B
ATOM	2755	0	LYS	1180	-14.092	-5.005	23.993	1.00 35.10	В
ATOM	2756	N	SER	1181	-15.934	-4.229	22.965	1.00 32.74	В
ATOM ATOM	2757 2758	CA CB	SER SER	1181 1181	-16.187 -16.910	-3.252 -2.045	24.003 23.421	1.00 33.42 1.00 36.08	B B
ATOM	2759	OG	SER	1181	-17.803	-2.468	22.401	1.00 30.03	В
ATOM	2760	C	SER	1181	-17.030	-3.888	25.084	1.00 31.49	В
ATOM	2761	0	SER	1181	-18.041	-4.539	24.810	1.00 30.03	В
ATOM	2762	N	VAL	1182	-16.590	-3.720	26.318	1.00 30.24	В
ATOM ATOM	2763 2764	CA CB	VAL VAL	1182 1182	-17.319 -16.457	-4.255 -5.254	27.441 28.222	1.00 29.79 1.00 28.87	B B
ATOM	2765	CG1	VAL	1182	-15.334	-4.534	28.908	1.00 20.07	В
MOTA	2766	CG2	VAL	1182	-17.303	-5.996	29.221	1.00 30.09	В
ATOM	2767	C	VAL	1182	-17.673	-3.048	28.302	1.00 30.76	В
ATOM ATOM	2768 2769	O N	VAL	1182 1183	-16.949	-2.035	28.293	1.00 30.66	В
ATOM	2770	N CA	ASN ASN	1183	-18.800 -19.266	-3.145 -2.068	29.008 29.873	1.00 29.22 1.00 26.49	B B
ATOM	2771	CB	ASN	1183	-20.751	-2.241	30.171	1.00 25.97	B
MOTA	2772	CG	ASN	1183	-21.287	-1.154	31.058	1.00 25.94	В
MOTA	2773	OD1	ASN	1183	-20.631	-0.139	31.265	1.00 26.14	В
ATOM ATOM	2774 2775		ASN ASN	1183 1183	-22.485 -18.488	-1.356 -2.059	31.595 31.178	1.00 26.47 1.00 25.98	В
ATOM	2776	C O	ASN	1183	-18.706	-2.039	32.051	1.00 25.60	B B
ATOM	2777	Ň	ALA	1184	-17.589	-1.095	31.318	1.00 25.72	B
ATOM	2778	CA	ALA	1184	-16.775	-1.010	32.516	1.00 25.10	В
ATOM	2779	CB	ALA	1184	-15.465	-0.289	32.198	1.00 23.98	В
ATOM ATOM	2780 2781	C O	ALA ALA	1184 1184	-17.497 -16.919	-0.322 -0.131	33.672 34.743	1.00 24.83 1.00 23.64	B B
ATOM	2782	N	ASP	1185	-18.762	0.045	33.464	1.00 23.64	В
MOTA	2783	CA	ASP	1185	-19.557	0.719	34.502	1.00 25.60	В
MOTA	2784	CB	ASP	1185	-20.621	1.600	33.855	1.00 24.94	В
MOTA	2785	CG OD1	ASP	1185	-20.064	2.925	33.385	1.00 26.22	В
ATOM ATOM	2786 2787		ASP ASP	1185 1185	-20.733 -18.957	3.594 3.305	32.574 33.830	1.00 26.83 1.00 26.39	B B
ATOM	2788	C	ASP	1185	-20.231	-0.201	35.522	1.00 26.43	В

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2789 2790 2791 2792 2793 2794 2795	O ASP N GLN CA GLN CB GLN CG GLN CD GLN OE1 GLN	1185 1186 1186 1186 1186 1186 1186	-20.378 -20.655 -21.287 -21.920 -21.002 -21.762 -21.660	0.168 -1.385 -2.326 -3.492 -4.238 -5.094 -4.895	36.687 35.089 35.998 35.230 34.305 33.307 32.097	1.00 27.46 1.00 26.01 1.00 24.85 1.00 25.72 1.00 25.02 1.00 25.24 1.00 24.55	
ATOM ATOM ATOM ATOM ATOM	2796 2797 2798 2799 2800 2801	NE2 GLN C GLN O GLN N PRO CD PRO CA PRO	1186 1186 1186 1187 1187	-22.529 -20.200 -19.017 -20.584 -21.959 -19.621	-6.049 -2.811 -2.538 -3.532 -3.913 -4.040	33.810 36.951 36.751 38.014 38.341 39.004	1.00 21.95 1.00 24.39 1.00 26.09 1.00 23.92 1.00 21.29 1.00 22.56	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2802 2803 2804 2805 2806 2807 2808	CB PRO CG PRO C PRO O PRO N LEU CA LEU CB LEU	1187 1187 1187 1187 1188 1188	-20.507 -21.872 -18.529 -18.747 -17.346 -16.236 -15.041	-4.780 -4.199 -4.932 -5.649 -4.891 -5.682 -5.586	40.004 39.803 38.415 37.443 39.012 38.512 39.461	1.00 24.86 1.00 24.58 1.00 22.14 1.00 20.75 1.00 22.47 1.00 26.58 1.00 26.72	
ATOM ATOM ATOM ATOM ATOM ATOM	2809 2810 2811 2812 2813 2814	CG LEU CD1 LEU CD2 LEU C LEU O LEU N GLU	1188 1188 1188 1188 1188 1188	-13.977 -14.552 -13.416 -16.584 -16.168 -17.348	-3.366 -4.539 -3.425 -3.965 -7.139 -7.702 -7.745	39.089 38.218 40.367 38.251 37.238 39.155	1.00 20.72 1.00 28.86 1.00 25.89 1.00 28.88 1.00 27.85 1.00 27.37 1.00 30.54	
ATOM ATOM ATOM ATOM ATOM ATOM	2815 2816 2817 2818 2819 2820	CA GLU CB GLU CG GLU CD GLU OE1 GLU OE2 GLU	1189 1189 1189 1189 1189	-17.745 -18.879 -20.198 -21.133 -20.742	-7.743 -9.146 -9.516 -9.905 -10.748 -11.169 -10.991	38.982 39.942 39.233 40.083 41.192 39.627	1.00 30.34 1.00 32.92 1.00 37.08 1.00 41.54 1.00 44.57 1.00 45.60 1.00 45.52	
ATOM ATOM ATOM ATOM ATOM	2821 2822 2823 2824 2825 2826	C GLU O GLU N ASN CA ASN CB ASN	1189 1189 1190 1190 1190	-18.261 -17.941 -19.043 -19.644 -20.749 -21.913	-9.321 -10.292 -8.346 -8.367 -7.319 -7.611	37.562 36.881 37.117 35.792 35.715	1.00 31.70 1.00 31.65 1.00 31.80 1.00 33.64 1.00 35.17	
ATOM ATOM ATOM ATOM ATOM	2827 2828 2829 2830 2831	CG ASN OD1 ASN ND2 ASN C ASN O ASN N VAL	1190 1190 1190 1190 1191	-23.064 -21.616 -18.602 -18.513 -17.852	-7.640 -7.820 -8.107 -8.865 -7.015	36.651 36.229 37.928 34.701 33.725 34.841	1.00 36.90 1.00 40.73 1.00 34.96 1.00 33.70 1.00 35.35 1.00 30.81	
ATOM ATOM ATOM ATOM ATOM ATOM	2832 2833 2834 2835 2836 2837	CA VAL CB VAL CG1 VAL CG2 VAL C VAL O VAL	1191 1191 1191 1191 1191 1191	-16.831 -15.849 -14.845 -16.621 -16.052 -15.827	-6.687 -5.626 -5.216 -4.432 -7.972 -8.269	33.858 34.427 33.363 34.938 33.515 32.341	1.00 29.71 1.00 28.83 1.00 27.90 1.00 25.92 1.00 29.17 1.00 28.36	
ATOM ATOM ATOM ATOM ATOM ATOM	2838 2839 2840 2841 2842 2843	N VAL CA VAL CB VAL CG1 VAL CG2 VAL C VAL	1192 1192 1192 1192 1192 1192	-15.708 -14.972	-8.751 -9.992 -10.684 -11.776 -9.699	34.545 34.359 35.687 35.425 36.671 33.546	1.00 29.21 1.00 30.67 1.00 30.86 1.00 30.14 1.00 30.01 1.00 32.39	
ATOM ATOM	2844 2845	O VAL N GLU	1192 1193	-15.434 -16.779	-11.256	32.379 34.168	1.00 32.39 1.00 30.84 1.00 33.20	

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	22222222222222222222222222222222222222	CA GLU CB GLU CB GLU CC GLU CD GLU CC	1193 1193 1193 1193 1193 1193 1193 1199 1	-17.592 -12.59 -18.878 -12.86 -20.023 -11.85 -21.244 -12.23 -21.158 -13.17 -22.294 -11.56 -17.924 -12.14 -17.712 -12.88 -18.386 -10.89 -18.737 -10.33 -19.166 -8.89 -20.659 -8.74 -21.333 -9.77 -21.178 -7.62 -17.562 -10.41 -17.722 -10.68 -16.380 -10.12 -15.166 -10.11 -14.098 -9.22 -13.181 -8.70 -13.326 -9.99 -14.675 -11.56 -13.952 -11.87 -15.124 -12.46 -14.739 -13.84 -15.030 -14.60 -14.757 -16.09 -13.447 -16.58 -13.187 -17.94 -15.806 -17.09 -13.447 -16.58 -13.187 -17.94 -15.806 -17.02 -15.552 -18.39 -14.244 -18.84 -14.020 -20.21 -15.507 -14.47 -14.917 -15.12 -16.825 -14.28 -17.693 -14.81 -19.105 -14.22 -20.091 -15.06 -19.537 -16.42 -19.363 -16.71 -19.247 -17.25 -17.144 -14.41 -17.065 -15.22 -16.760 -13.14 -17.065 -15.22 -16.760 -13.14 -15.070 -14.22 -20.091 -15.06 -19.537 -16.42 -19.363 -16.71 -19.247 -17.25 -17.144 -14.41 -17.065 -15.22 -16.760 -13.14 -15.097 -10.36 -15.297 -10.36 -15.297 -10.36 -15.297 -10.36 -15.297 -10.36 -15.297 -10.36 -15.3937 -13.39 -13.987 -13.98 -13.987 -13.98 -13.984 -14.69	6 34.295 0 34.197 0 35.889 34.929 35.889 34.929 31.100 31.927 30.625 30.768 30.768 30.768 30.677 9 30.677 9 30.677 9 30.032 29.061 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 29.342 20.342 20.342 20.342 20.342 20.342 21.433 21.062 22.7.716 23.31.062	1.00 36.11 1.00 43.09 1.00 46.41 1.00 47.71 1.00 45.13 1.00 36.07 1.00 36.07 1.00 36.05 1.00 37.45 1.00 38.47 1.00 38.47 1.00 38.47 1.00 35.69 1.00 37.76 1.00 37.76 1.00 37.71 1.00 37.72 1.00 57.82 1.00 57.72 1.00 57.72 1.00 39.80 1.00 37.71 1.00 39.80 1.00 37.71 1.00 39.80 1.00 37.74 1.00 31.47 1.00 31.50 1.00 31.47 1.00 31.50 1.00 31.50 1.00 28.68 1.00 24.35	***************************************
					4 25.867 8 25.462 7 26.075		

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ATOM 2939 CD2 LEU 1203 -8.435 -18.036 21.984 1.00 29.77 ATOM 2940 C LEU 1203 -11.920 -19.686 20.428 1.00 35.15 ATOM 2941 O LEU 1203 -11.222 -20.656 20.137 1.00 37.00 ATOM 2942 N GLU 1205 -13.240 -19.688 20.313 1.00 38.14 ATOM 2943 CA GLU 1205 -13.936 -20.870 19.847 1.00 40.88 ATOM 2944 CB GLU 1205 -15.268 -21.024 20.592 1.00 41.71 ATOM 2945 CG GLU 1205 -15.268 -21.024 20.592 1.00 41.71 ATOM 2946 CD GLU 1205 -15.246 -22.049 21.733 1.00 42.35 ATOM 2947 OE1 GLU 1205 -13.858 -22.268 22.326 1.00 45.00 ATOM 2947 OE1 GLU 1205 -12.876 -22.379 21.559 1.00 47.85 ATOM 2948 OE2 GLU 1205 -13.740 -22.340 23.569 1.00 44.55	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2903 2904 2905 2906 2907 2908 2910 2911 29113 2914 2915 2917 2918 2919 2921 2922 2923 2923 2923 2923 2933 293	CONCABCG11 CONCABCGCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	ILE ELLE ELLE LLE LLE LLE LLE LLE LLE LL	1199 1199 1200 1200 1200 1200 1200 1200	-8.517 -13.627 16.994 1.00 38.43 -12.825 -16.873 19.807 1.00 30.13 -12.571 -17.308 18.681 1.00 29.33 -12.269 -17.331 20.922 1.00 30.06 -11.295 -18.409 20.944 1.00 31.23 -10.823 -18.641 22.370 1.00 29.49 -9.648 -17.820 22.877 1.00 29.98	
ATOM 2930 CZ TYR 1202	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2920 2921 2922 2923 2924 2925 2926 2927 2928	C O N CA CB CG CD1 CE1 CD2	LYS LYS TYR TYR TYR TYR TYR TYR	1201 1201 1202 1202 1202 1202 1202 1202	-15.748 -16.789 21.049 1.00 34.21 -16.084 -17.351 20.012 1.00 35.71 -14.684 -16.005 21.139 1.00 32.69 -13.813 -15.737 20.004 1.00 32.06 -13.059 -14.429 20.249 1.00 32.04 -11.845 -14.249 19.386 1.00 33.32 -11.967 -13.778 18.080 1.00 34.25 -10.858 -13.579 17.284 1.00 35.32 -10.570 -14.520 19.874 1.00 33.61]]]]]
ATOM 2940 C LEU 1203 -11.920 -19.686 20.428 1.00 35.15 ATOM 2941 O LEU 1203 -11.222 -20.656 20.137 1.00 37.00 ATOM 2942 N GLU 1205 -13.240 -19.688 20.313 1.00 38.14 ATOM 2943 CA GLU 1205 -13.936 -20.870 19.847 1.00 40.88 ATOM 2944 CB GLU 1205 -15.268 -21.024 20.592 1.00 41.71 ATOM 2945 CG GLU 1205 -15.246 -22.049 21.733 1.00 42.35 ATOM 2946 CD GLU 1205 -13.858 -22.268 22.326 1.00 45.00 ATOM 2947 OE1 GLU 1205 -12.876 -22.379 21.559 1.00 47.85	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2930 2931 2932 2933 2934 2935 2936 2937 2938	CZ OH C O N CA CB CG CD1	TYR TYR TYR TYR LEU LEU LEU LEU LEU	1202 1202 1202 1202 1203 1203 1203 1203	-9.604 -13.851 17.790 1.00 34.45 -8.517 -13.627 16.994 1.00 38.43 -12.825 -16.873 19.807 1.00 30.13 -12.571 -17.308 18.681 1.00 29.33 -12.269 -17.331 20.922 1.00 30.06 -11.295 -18.409 20.944 1.00 31.23 -10.823 -18.641 22.370 1.00 29.49 -9.648 -17.820 22.877 1.00 29.98 -9.356 -18.234 24.301 1.00 30.87	F F F F F F
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2940 2941 2942 2943 2944 2945 2946 2947	C O N CA CB CC CD OE1	LEU LEU GLU GLU GLU GLU GLU GLU	1203 1203 1205 1205 1205 1205 1205 1205	-11.920 -19.686 20.428 1.00 35.15 -11.222 -20.656 20.137 1.00 37.00 -13.240 -19.688 20.313 1.00 38.14 -13.936 -20.870 19.847 1.00 40.88 -15.268 -21.024 20.592 1.00 41.71 -15.246 -22.049 21.733 1.00 42.35 -13.858 -22.268 22.326 1.00 45.00 -12.876 -22.379 21.559 1.00 47.85	E E E E E

Fig. 2A-51

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В B B В В В В В В В

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В В

ATOM	2960	N ILE	1207	-12.408	-19.983	16.161	1.00 45.64
ATOM	2961	CA ILE	1207	-11.135	-20.119	15.477	1.00 46.49
ATOM	2962	CB ILE	1207	-10.142	-19.011	15.934	1.00 44.67
ATOM	2963	CG2 ILE	1207	-10.858	-17.668 -19.319	15.945	1.00 42.99
ATOM	2964	CG1 ILE	1207	-9.578		17.326	1.00 43.35
ATOM	2965	CD1 ILE	1207	-8.372	-18.477	17.695	1.00 40.56
ATOM	2966	C ILE	1207	-10.546	-21.505	15.731	1.00 49.19
ATOM	2967	O ILE	1207	-9.765	-21.303	14.926	1.00 49.19
ATOM	2968	N ARG	1208	-10.933	-22.126	16.847	1.00 51.37
ATOM	2969	CA ARG	1208	-10.446	-23.455	17.199	
MOTA	2970	CB ARG	1208	-9.957	-23.435 -23.495	18.653	1.00 53.73 1.00 55.52
MOTA	2971 2972	CG ARG	1208	-9.969	-24.896	19.281	1.00 58.37
ATOM	2972	CD ARG	1208	-8.666	-25.619	19.007	1.00 61.49
ATOM		NE ARG	1208	-8.248	-26.502	20.100	1.00 65.11
ATOM	2974	CZ ARG	1208	-7.068	-27.113	20.161	1.00 66.79
ATOM	2975	NH1 ARG	1208	-6.188	-26.934 -27.892	19.185	1.00 67.81
ATOM	2976	NH2 ARG	1208	-6.779		21.189	1.00 68.01
MOTA	2977	C ARG	1208	-11.576	-24.452	17.011	1.00 53.91
ATOM	2978	O ARG	1208	-11.642	-25.123	15.983	1.00 55.37
ATOM	2979	OH2 TIP3	500	37.299	9.800	4.044	1.00 37.63
MOTA	2980	OH2 TIP3	501	38.757	11.999	6.275	1.00 18.09
ATOM	2981	OH2 TIP3	502	43.991	17.954	3.473	1.00 33.76
ATOM	2982	OH2 TIP3	504	39.230	32.411	4.691	1.00 46.51
MOTA	2983	OH2 TIP3	506	34.991	22.293	17.555	1.00 23.59
ATOM	2984	OH2 TIP3	507	22.200	9.651	16.956	1.00 17.69
ATOM	2985	OH2 TIP3	508	30.284	17.100	19.446	1.00 25.84
MOTA	2986	OH2 TIP3	509	15.592	-7.199	18.885	1.00 43.65
ATOM	2987	OH2 TIP3	510	20.407	15.347	15.916	1.00 27.65
ATOM	2988	OH2 TIP3	511	13.022	4.354	-2.732	1.00 57.50
MOTA	2989	OH2 TIP3	512	16.001	-1.210	0.176	1.00 58.45
ATOM	2990	OH2 TIP3	513	4.718	11.821	7.123	1.00 47.25
ATOM	2991	OH2 TIP3	514	16.004	24.440	9.316	1.00 35.29
MOTA	2992	OH2 TIP3	515	29.581	9.912	-8.341	1.00 6.39
ATOM	2993	OH2 TIP3	516	30.422	4.262 3.080	-7.153	1.00 28.66
ATOM	2994	OH2 TIP3	517	30.100		-11.171	1.00 58.91
MOTA	2995	OH2 TIP3	518	20.652	1.190	-1.526	1.00 25.86
ATOM	2996	OH2 TIP3	519	27.470	2.321	-5.485	1.00 26.21
ATOM	2997	OH2 TIP3	523	-4.307	-2.443	21.738	1.00 28.13
MOTA	2998	OH2 TIP3	525	-0.578	17.057	27.555	1.00 32.90
ATOM	2999	OH2 TIP3	526	34.800	9.578	5.796	1.00 23.73
ATOM	3000	OH2 TIP3	528	32.545	23.778	17.866	1.00 33.02
ATOM	3001	OH2 TIP3	529	42.307	23.527	4.997	1.00 44.19
ATOM	3002	OH2 TIP3	530	31.702	29.905	17.688	1.00 36.41
ATOM	3003	OH2 TIP3	534	14.238	16.302	26.327	1.00 27.51
MOTA	3004	OH2 TIP3	535	21.111	36.027	17.890	1.00 35.07
ATOM	3005	OH2 TIP3	536	17.977	16.366	3.734	1.00 29.01
ATOM	3006	OH2 TIP3	537	29.610	5.124	8.888	1.00 45.45
ATOM	3007	OH2 TIP3	538	17.608	-3.137	0.196	1.00 45.25
ATOM	3008	OH2 TIP3	539	5.670	8.591	4.143	1.00 41.64
ATOM	3009	OH2 TIP3	541	4.763	4.486	9.124	1.00 39.02
ATOM	3010	OH2 TIP3	542	8.207	22.430	10.831	1.00 42.81
ATOM	3011	OH2 TIP3	543	15.118	25.044	5.498	1.00 44.03
ATOM	3012	OH2 TIP3	544	29.511	10.901	-10.894	1.00 39.37
ATOM	3013	OH2 TIP3	545	32.473	0.324	-8.592	1.00 36.37
ATOM	3014	OH2 TIP3	546	35.074	-1.173	-5.291	1.00 24.33
ATOM	3015	OH2 TIP3	547	32.326	-0.577	-3.088	1.00 45.29
ATOM	3016	OH2 TIP3	548	19.617	5.436	-6.168	1.00 46.42

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	30189 01789	OH2 TIP3	901235690123456789123678012345678901345701234568901234 555555555555555555555555555555555555	20.033
ATOM	3067	OH2 TIP3	611	25.495 -6.170 1.847 1.00 53.33
ATOM	3068	OH2 TIP3	612	32.114 -3.720 -5.524 1.00 48.53

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ATOM ATOM	3074 3075	OH2 TIP3 OH2 TIP3	624 625		6.414 8.152	-8.147 -11.615		23.12 24.45
ATOM ATOM	3076 3077	OH2 TIP3 OH2 TIP3	626 628	-2.622 1	1.332 9.633		1.00	43.49 37.19
MOTA MOTA	3078 3079	OH2 TIP3 OH2 TIP3	629 630		7.361 0.515	39.889 37.881		61.00 31.55
ATOM ATOM	3080 3081	OH2 TIP3 OH2 TIP3	631 632	-10.217 -	1.307	39.597 35.049	1.00	
ATOM	3082	OH2 TIP3	633	0.406 - 2	4.863	30.031	1.00	49.55
ATOM ATOM	3083 3084	OH2 TIP3 OH2 TIP3	634 635	14.511 -	5.021 7.526	23.436 33.274	1.00	
ATOM ATOM	3085 3086	OH2 TIP3 OH2 TIP3	636 637		3.257 1.130	23.832 33.912		30.58 48.46
ATOM ATOM	3087 3088	OH2 TIP3 OH2 TIP3	638 639	5.491 -	0.955 5.224	33.749 27.892	1.00	49.13
MOTA	3089	OH2 TIP3	641	9.121 1	1.477	29.216	1.00	41.58
ATOM ATOM	3090 3091	OH2 TIP3 OH2 TIP3	642 643	13.139 -	7.427 9.763	14.592	1.00	44.59 39.50
ATOM ATOM	3092 3093	OH2 TIP3 OH2 TIP3	644 645	8.918 -1	5.955 9.436		1.00	29.03 58.43
ATOM ATOM	3094 3095	OH2 TIP3 OH2 TIP3	646 647		2.468 2.822	17.407 16.942		37.35 37.73
ATOM ATOM	3096 3097	OH2 TIP3 OH2 TIP3	648 649	4.341 -2	2.047	14.464 13.642	1.00	48.23 33.18
ATOM	3098 3099	OH2 TIP3	650 651	1.353 -2	5.194 9.824	20.926	1.00	51.00
ATOM ATOM	3100	OH2 TIP3	653	1.940 1	4.682	23.109	1.00	58.49
ATOM ATOM	3101 3102	OH2 TIP3 OH2 TIP3	655 656	6.059 -	4.362 1.930	10.276 9.076	1.00	38.36 26.19
ATOM ATOM	3103 3104	OH2 TIP3 OH2 TIP3	657 659		1.127 3.734			50.53
ATOM ATOM	3105 3106	OH2 TIP3 OH2 TIP3	661 662	-16.640	6.818 9.011	28.144 30.213	1.00	25.26 47.61
ATOM ATOM	3107 3108	OH2 TIP3 OH2 TIP3	664 665	-17.949 13	3.378	32.218 44.264		36.07
ATOM	3109	OH2 TIP3	666	-8.590 20	0.473	43.414	1.00	42.81
ATOM ATOM	3110 3111	OH2 TIP3 OH2 TIP3	667 668	-11.938 2	4.339 6.641	41.537 38.313	1.00	53.87 40.91
ATOM ATOM	3112 3113	OH2 TIP3 OH2 TIP3	669 670		2.520 2.073	38.617 41.400	1.00	49.06 33.81
ATOM ATOM	3114 3115	OH2 TIP3 OH2 TIP3	671 672		4.658 7.317	41.524 39.288	$1.00 \\ 1.00$	48.57 62.04
ATOM ATOM	3116 3117	OH2 TIP3 OH2 TIP3	675 676	-10.916 1	7.235	28.973 29.928	1.00	19.60 44.23
ATOM ATOM	3118 3119	OH2 TIP3 OH2 TIP3	677 678	-12.376 1·	4.997	26.011 22.910		25.27 36.08
MOTA	3120	OH2 TIP3	679	-15.130 -13	2.373	21.294	1.00	31.35
ATOM ATOM	3121 3122	OH2 TIP3 OH2 TIP3	680 681	-24.281 -	2.963	29.740 32.226	1.00	53.82
MOTA MOTA	3123 3124	OH2 TIP3 OH2 TIP3	682 683	-16.683 -	7.204 3.185	29.606 41.795	$\frac{1.00}{1.00}$	40.17 24.03
ATOM ATOM	3125 3126	OH2 TIP3 OH2 TIP3	701 702	37.640	1.019 5.709	7.364 5.316		54.16 52.52
ATOM ATOM	3127 3128	OH2 TIP3 OH2 TIP3	705 706	19.919 -	7.084 9.970	13.950 26.417	1.00	54.40 47.37
ATOM ATOM	3129 3130	OH2 TIP3 OH2 TIP3	707 708	24.320 2	1.898 8.372	25.471 29.036	1.00	55.75 36.22

Fig. 2A-54

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Fig. 2A-55

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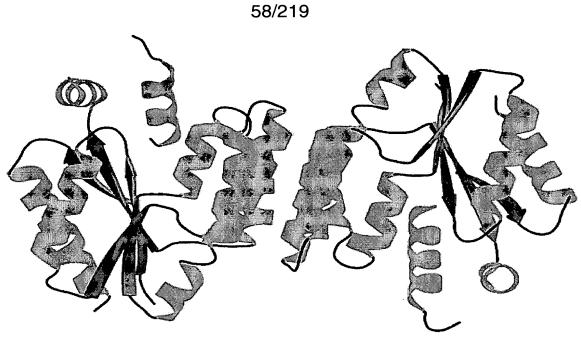
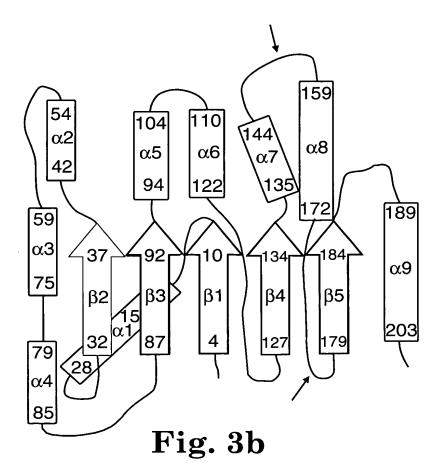
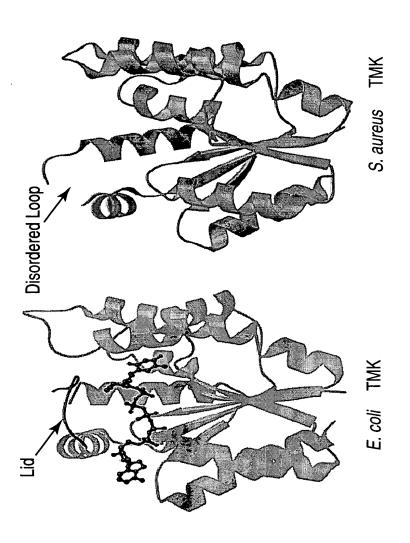


Fig. 3a



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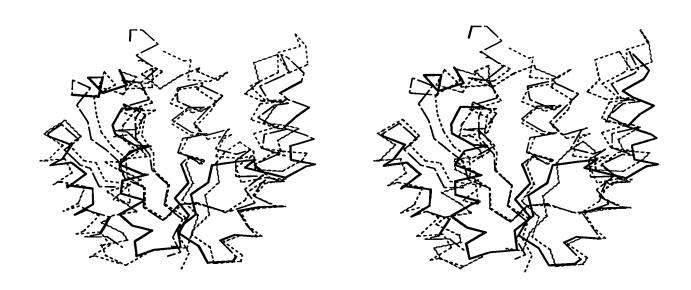


Fig. 5a

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		51	rslvldiksvgdevitdkaevlmfyaarvqlvetvikpalangtwvigdr	100
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		94	YIDSSLAYQGYARGIGVEEVRALNEFAINGLYPDLTIYLNVSAEVGRERI	143
	1	0.1		1 4 0
	1	LUI	hdlst qayqgggrgid qhmlatlr davlgdfrpdltlyldvtpevglkr.	149
	1	111	IKNSRDONRLDOEDLKFHEKVIEGYOEIIHNESORFKSVNADOPLENVVE	103
	7	. 4 4	: : . : : : . :	193
	1	50	arargeldriegesfdffnrtrarylela.agdksihtidatgpleavmd	198
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	1	194	DTYOTIIKYLEKIRSHHHHHH 214	
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	1	99	airttythwykelda 213	

Fig. 5b

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Fig. 6a

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Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1 Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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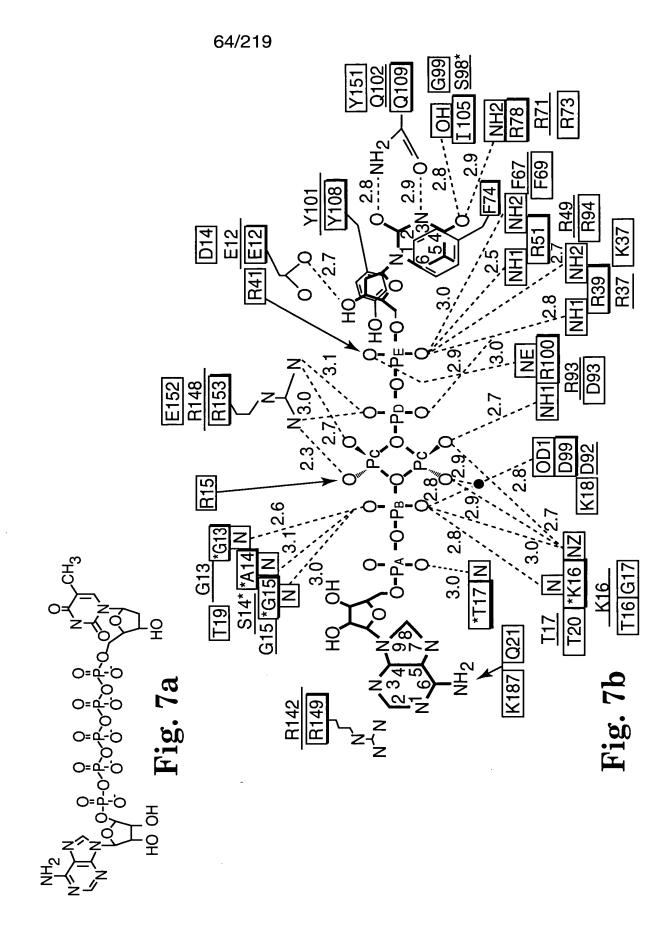
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	149	DQNRLDQEDLKFHEKVIEGYQEIIHNESQR.FKSVNADQPLENVVEDTYQ : . : : .:: .: .!: :::	197
	148	${\tt deryetvkfqekvkqtfmklldkeirkgdesitivdvtnkgiqevea}$	194
	198	TIIKYLEKIRSHHHHHH 214	
	195	liwaiyanylathidhdkfaff 216	

Fig. 6b

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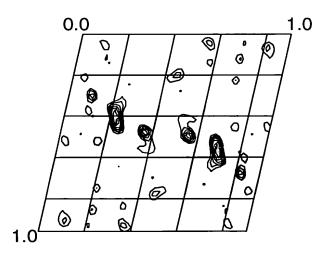


Fig. 8a

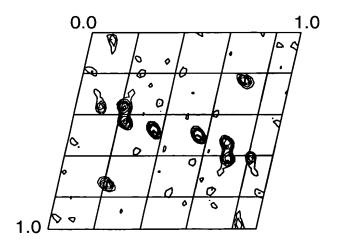


Fig. 8b

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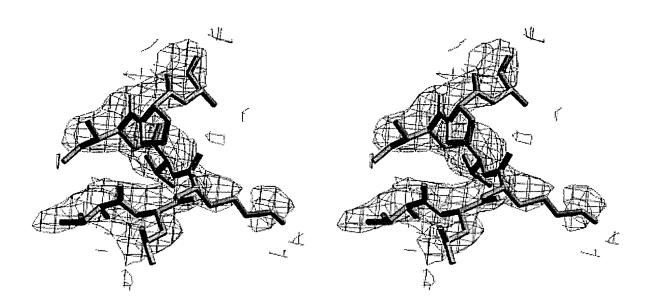


Fig. 9a

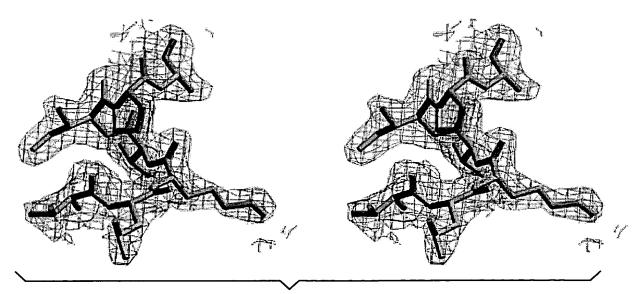


Fig. 9b

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1 Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1 Express Mail No.: EV 073687660 US

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Fig. 10A-4

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE **Applicant(s):** Timothy E. Benson **Serial N**: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) **D** cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Serial No.: Unassigned (Parent: 09/632,553)

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Perent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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РРРР РРР РР

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE **Applicant(s)**: Timothy E. Benson **Serial No.:** Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) **D** cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Perent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Fig. 10A-14

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-15

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Fig. 10A-17

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
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Fig. 10A-20

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

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Fig. 10A-23

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Fig. 10A-24

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOGOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

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Fig. 10A-27

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Fig. 10A-28

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mall No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-29

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOGOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-30

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOGOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

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Fig. 10A-33

Express Mall N .: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1 Express Mail N .: EV 073687660 US Sheet 102 of 219

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Fig. 10A-35

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson

Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)
Express Mail N .: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-37

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE **Applicant(s)**: Timothy E. Benson **Serial No.**: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) **Docket**: 6245.N DV1

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Fig. 10A-39

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Fig. 10A-40

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-41

Express Mall N .: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-42

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mail N .: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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43445646462042813009920648860100759048783079010792790356722783651474957 74860830493524499000986090006007000975995780900995181909988979999898750993

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOGOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mail N .: EV 073687660 US

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68174787959994651435756810462652628732762491473949355638149741972192481

Fig. 10A-44

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE

Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Express Mall No.: EV 073687660 US

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Filed: Herewith (Parent: Aug. 4, 2000)

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail N .: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
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Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

D cket: 6245.N DV1 Sheet 114 of 219

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE **Applicant(s)**: Timothy E. Benson **Serial N** .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1 Express Mail No.: EV 073687660 US Sheet 116 of 219

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Fig. 10A-49

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Fig. 10A-50

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mail N .: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-52

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
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Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

Express Mall N .: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)
Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

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Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mall N .: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Express Mall No.: EV 073687660 US

D cket: 6245.N DV1 Sheet 127 of 219

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

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Fig. 10A-61

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Titie: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

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335943982146657520783847435818826726929383998950853127370507659239996660 99371120998939989963000000000000000000000000000

Fig. 10A-68

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1 Docket: 6245.N DV1 Express Mall No.: EV 073687660 US Sheet 137 of 219

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Fig. 10A-70

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

Express Mall No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mall No.: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOGOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-77

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Fig. 10A-78

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Fig. 10A-80

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Fig. 10A-81

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Fig. 10A-90

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Fig. 10A-91

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310979982232740556187969588003982455498639345039169206269749013393567383 53589990875273737300915888035063453120486888064697357185964533676164602769285 545003524116679550318845931439333168990568295097139066078686604027580728 2211111 122333311 1312 21 1222133122 3112 11532111115 31 1 231522223221
= = = = = = = = = = = = = = = = = = =
9052007960097745762784732180-1248669054-10758758022000147170770270299221527 2075986561-101-122242570764824-111-147328286796101-12447-1028745073-1-170-1222234
= = = = = = = = = = = = = = = = = = =
444925729633528831581989173845736543693794817112086914153151237366578845 7.3169094939305065280598754824053814936093496753880606148869727244488051679 55914596495491454010127426 170779181814382324353223934680002225252 70186 1 1 113213 113 21311 1 3 32 11 1131122 3 32 321212 321 3 33 21321
6864588590088720297451155559640738094162525872904418062277840965487872770211210700999891581605140999790904905103009999999139091072009999577089383

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NO
666667777777777777777778888888888888888
23456012345678901234501234567890123450123456789012345012 111111 1111111 1111111
88844838317874444978553722552159691017988359271988365704431189983171119975 06155166786332831486664713229108794842644573706867250974053816012556350 2 1 22221 1213111 2231111323 11 1 1 212 212
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49604333318883777340710944419560449728381418519957054809744635084493885097 45715111112684242764493111334223264692152725222020863778212413259626365211 1 32 1
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245532001209601001307917484082743310848029260217187025540812733983140994 0625075305578215617879534888823308669052983832504255774306299467975376303 9731621233705685320545644091518145262008210 1534444440092333626460350 53 22 21 1 231221132 112 11 122212212 23 3 3 12112 1313232222122 33
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91073738643613001376378609708565019252669078835064974764436839836324966 311100968690288994550049808681289144008581957571654210999698500153841987

Fig. 10A-94

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22222222222222222222222222222222222222
345678901234501234567890123456789012345012345678901234567890123461234567890 1111111111111111122222222222222223333333
047304921500875551919020438957785129677964999464848834896301485224434512 047304921500875551919020043895778512967796499946484883489630148522448512 971044007430298841431562278884655948500749581032862927634090445979122685 211101261196595395205237935607486752274796644153355542878583751774713949 11113415311 1 12 2111363311 1 21 11212 1 1 122211132211211 222113221
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8007500488337386852568791924218050905377777941965748295122010417568708234 3441152264450113144311125517112452423287415821112231224434656111222222231
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422758296283-152187240690157310071950847498883419829204868633204360270247  1063149453141843316510327907801240558323009475008417895235274155496755860  49563 424471746831467931071899761419115474910817 87857694874623797192015  313 2 21311 1312213 211313 222 311333 13113131 1 12 311311 2221221 1
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75945504762678333495600660033728176964132696675849725373381225062939622779199506350509999899709722010999989799811406109999878878596820409115888974

Fig. 10A-95

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770.867.151.161.757.301.311.0460.3661.737.97.667.847.71334207.58150.759.82957.36469.857.8662.46240.263641.875.750.3966.3966.26240.26365443.939.308.8461.44446.295.039.663.303.303.303.303.303.303.303.303.303
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86125955729624118755766138716853204514523566448663856087293154092461527 59124125123456048623511521145220173622112326364901114133228634221213221 11 2 21 4 21 1 1
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6455239999401327544037796914915873715710256196532224253120562660375288701 05873923980970630672359386498199307618201824191079163447313421852447591 29813485545230 066946382608643150161659745 2916191848277891080991240936 121 3111 1122 21 1 121322 1 1132123 21133 113 2 22 1 2 13122211 1212
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46876512594539140171735297878576248396489311051272145939477195164945912 42207991984424210205377199724711004899187925221099941756820830858939826 

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$Q_{N}(N) = \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \right) + \frac{1}{N} \left( \frac{1}{N} \right) + \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \right) + \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \right) + \frac{1}{N} \left( \frac{1}{N} \left( \frac{1}{N} \right) + \frac{1}{N} \left( \frac{1}{N} \right) + \frac{1}{N} \left( \frac{1}{N} \left$
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06700237403043037300490448859244406766182795682216588878411973910414275612 818268148151575697984919600066979268804353256716349957954392648446445772 218127739346676688758 484777255593596884448881341205063859 88516026192601 2221 32 31212 1112 2 3121 1 3 11 12 2 2211 3311
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17572507250118982945729618403310279506063600993844698973749713122866265 20249999856624100899087593140058898287507207014211218178971933131998669 

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6666667777777777778888888888889999999999
67890012345678901234567801234567012345601234501234010123456789012345601 11111111
60315252575888834041250868868147755466065982770039357513482365952332464348 6031525252575888834041250868868147755466065982770039357513482365952332464348 6031525252548388232464348 60315252555888324174868884505488827558970048837 688649041903188076388025204475556403417340554164075458884505483827558970048837 3330729406925997748832417436555541149923190776744440780934020254134130815626 4222212 2111 1 1 222111 2111 11 11 11 1 1 2323132211 1 211
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648277797682778124608165670079072555755006468620006117556607977692176058065 12228112224926752124747222227924461775500642562787455554757021228245066122711 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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9414525919728663380142254538984137774035913174202886200000000000000071 559201781579136241082595521524531743181320577675470300000000000000002 26 063745317526026932585 361702414249 3130922824355678 88 8 88 8 88 68 31 2 11 3131 3213 2323 2 1 213312 12 12311 1223333211 11 1 1 1
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455921095023429768548832343058151795555158978158206667000404056115322251 99972918996492469996860025920221276850178058087101183040060901200000000000000000000000000000000

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27456789012745601274567890127450127456789012745012745678901274567 1111111 1111111
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191532089128880182799925214706648110523495970766917774985417316795238259. 62260647227303560733021565796792695127694292662971398351686858046243501 75220237738938866918490628508455435217955106481606920354920757960988130 37312211 2112 124511 1 4 1211 23312121323 131 1111111 3311 3423 121
= = = = = = = = = = = = = = = = = = =
90397504248489060835699199268510841419045865799950972891949309310219237 01132254245530211012359010645664411151325242617025134435822564411114426
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505581935963374361302384110993304925068769505195394984122345406212853878 69982726038581790868843019468779752653224007467492340815754650865335089 0340021891220434723729150479624 211291675952394650287930 34585383968170 3 22113113321 2 2 212 231 21 32 213122132233112 3 2 221 3 2 2 3 11 12
======================================
300896923280775099982575263857454239800479221036063767917514926476890116 940872511203300099982421914732083899598857291000849377246248200099997994

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92251540762122005115133997737676113342157430676934752694411052079219703546 3.4963182332064312322599822329744280130372229557882231211137962503182279427263 533496519888112250247065546039662458555631409097696848106424236077798291474 12111 1 113112122221111 1311 11 14111111132 11 12112311 14 11 11322111
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= = = = = = = = = = = = = = = = = = =
928288822796255978288164440832526440539014610535042461101164349835694730 3.67468773801325477081237031963670342255391138914124281814947534106045 3580225265932965750764 90414452532624245340631774759212 30932106045 700 33 31 13 222 1121 22 1 23 332131 231 212 212 221 2 131 211 3212211 131
= = = = = = = = = = = = = = = = = = =
348360238684546634807608622074594603629720800793220214840564888832323570 82000120199879114961401099955220251044019084921974422431087883099492201

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) 1 ) 2 ) 3
2 122321211 1 11 1 122133 1 111 1 11144311 2 12 2223 12211 1 1131 1
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957992875505416260729461007062142508657055296129486581785776846297246876 4214722126748180924255422721670021577311265178821612218657266652271267
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957199931469521050725217841713789864963416511267112878688813557341503613 8388253146239509083805543502903474811069755243556655713929405955986741939 96779122666603310898479588 5224825474 3163595476219270015322212841229173 22222 2 12 1332 122 21 1 1 1 1213323 1222123 2111 323331 31 112 11 2
= = = = = = = = = = = = = = = = = = =
27917626328888212477688652165135541722441771766326967140182803466590053432 09949959966221100986100844981120098898539920290199799991278815022859828 00000000000000000000000000000000000

Fig. 10A-101

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<i>ຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓຓ</i>
44444445555555555555555666666666666666
890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123
619644058805153030454510670205655414437741191302887813682854862254215003
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71021719017171162552785596159725471200071720575877677519727551769
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04836671565523600054167494761480003918928144990981567649162569947105874023 58474723854858447047186882188089820470870948995927823197275975918081373 24422405 91985305162114488043401272269 3150 8948334768095010298424546865 2322 23 12 3233 213 1 2233223212 21 2132 12232 11212 2 23213 1212222
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631310280625993167928890039473803645585057787009272464942342558379340455

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896905465662309364168124987829151792775600361759855054515254847480539998 145096647977466130647291788231411906688827174678694416336070002034165090 08917852147683883710463970184625053122528772244335781643422651852615739643 2 11 1322 11421 21 2112121 2 1 11322221 121 11 22 1111131111112 221
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07138834829464427647650148423740177406596482908750801991577402736589153
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31656356964148845399006908337699949458554888253419526045499469302920055875 53126009593749002441976951610421038927234775128459522741186098159100998 00000000000000000000000000000000

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64548999191309719819465971724581955092517772548898803399477774489909375844 675757599465566199888823808808104641488465359048189605942596362244994849511158 948869345469148850088322686089158883944808841753652068784314862535737737534735 1 1 2 32 31 11 22 11 111 1 2 2 2 21 1 13 1 1 1 1
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611488836904093201230151651719939714702186851716710800592055856800717670 20368549728512695521228535653256352272582284873176273130353137416932037 1 1 1 2 2 2 121
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194692858210594289688456329979208092225443234100567490726367600000000000000000000000000000000
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06251801446817925999474913953933569347558222388707417833662270247673144955

Fig. 10A-104

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89012340123456789012345012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789001234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890101234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890124567890124567890101234567890101245678901012456789010124567890101000000000000000000000000000000000
45986085445413017327476497787653435895461603203811111198966467477863938 2063839997956550219854484037211548144055009972971580368284060481716636796 11075688609668457191569925641666222253449509991796802888776666943648600164 22331 383121 22222 4 3421122223311 3352 1122211 111 111211211
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610080907170790648019911511196409679510111990480784080958311655698131015 46407541012000494040545999-15112073007803761616110154320091010701206434424659830 1021 11 1
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11850140074533376688035079400636555524429180208029141611520964010551400520 507001000999402296428010660999989828000008060819935500121009986422653422111

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1331-161-0305907817-1538000065816300388065304676300014761120146042945574346 21120146605211-243222377123322655482421409623122430324768191127212
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442343899571223553403911433968833719165745966612317201341585539626032944 9988815340261130173597893632213032775241338001009198941297010009091739

Express Mail No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-107

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Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Express Mall N .: EV 073687660 US

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95033374179511851608125302608235604313227168460359452703734171106062874 79901370087441163611400105968227522071059457413231731192983896517112027 

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5399077244003226412605384310419631834926725662969710262785570445117322963 887499581114069955169619110034913519510110098899339661410090899927420220

Fig. 10A-113

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail N .: EV 073687660 US

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0868141467358701058388821864085611695194405622788449768498048109130069882584867379498231813524469236034417221158137755836867881942595354677406998852698647547888428654887028200055606854346285686659501888870724974111462221111 1 2244 122 12223111211 1 23 333 11 1 3 231 1 233211
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10926480083305535136220786011000051388577294631787206853156874858790973 2430660159772941847926425244084947018242216645097845570422251534268904460 2278881557 209537359235083733102006727575823355568422445594554860900108136 2 2 11331 221 2121 113 2 213 112 1221 312212 3131331 131 21 21231112
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51891415997534764581450746690682384397417373016140511205238972826427428789999978810000000000000000000000000000

Fig. 10A-114

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87672166238157548340802196898297815693865939377811258048131227889195316 8107519823311115000909356701302773051114009868322410834121310594247620166 

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

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458089547212057012227620351998484833952864164024797677088212720924124598 248396488296835034342355944136315233722763423212428742449667121179437862 31 1 2
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Express Mall No.: EV 073687660 US

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261253739310134935038816930985595283919557581892314282828914727600835 7349507343938172714408339160637078366234624338631221884427479960053078444 374310894131189585078985254664664649415463634476233042869914416153778832 2122 2 2 123 22 1 31 2 1 121 1 31 2 231121322211 12 2 1 21 33 23 1221
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9355353666113333712726148921631177393147426689139104915378836116173969882 61000988149792012100299428275160130399914080381110969940798901220678974

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mall No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-118

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mall No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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6888759884647293665005257675906828567498731986574920611348579452718405080 3055023099823674622000524961571111000977584603111149612192722409061939513

Fig. 10A-119

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)
Filed: Herewith (Parent: Aug. 4, 2000)
Docket: 6245.N DV1

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Fig. 10A-121

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-123

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

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31028037513391265464397317356642527591374659823811514530145735281730022 9769158011116642058861210888982421100099998361001409724164000098784231

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

Express Mall No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

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Fig. 10A-126

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail N .: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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Fig. 10A-127

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mail N .: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

Express Mall N .: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Fig. 10A-130

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mail N .: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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73186564467827659323056635360912185305375122340701924436829066397885128

Fig. 10A-132

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE **Applicant(s)**: Timothy E. Benson **Serial No.**: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) **Docket:** 6245.N DV1

Express Mail N .: EV 073687660 US

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Fig. 10A-133

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

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Express Mail No.: EV 073687660 US

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32269251408989399118123264122282112219742049368301713389423563207743917 152101085701030001500011001511511110007783680200100399922000000000000000000000000000

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

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Fig. 10A-138

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

Express Mail N .: EV 073687660 US

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Fig. 10A-139

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Fig. 10A-140

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Perent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mall No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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38439128520958168412267310620439715423311526145014962832425158037202565 01324210000822302140745102101690002300711220111022000000000000000000000

Fig. 10A-141

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

Express Mail No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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31711273016317141328311398072834922473823842760252616624182967374097732 042110192010011203000000000000000000000000

Fig. 10A-142

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial N .: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

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367732594653390843032812816365478132348133107134958703471713698284088178 1111100755621310097246110400189105000803074111002220210400519001010400100

Fig. 10A-143

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOGOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

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23923009922184266888436369321449647130179481626608234133772861515362706757102221001002310002000000000000000000000

Fig. 10A-144

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

Express Mail No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

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12163172019453956512987507285916355521252586922936363044499816113866950101020010100130310401102000000000000000

Fig. 10A-145

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

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112095077944768353364718542243576232347448837944535162425251 2102612100401011203121013010011110040100700472030012070410

Fig. 10A-146

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOGOCCUS AUREUS* THYMIDYLATE KINASE **Applicant(s)**: Timothy E. Benson **Serial No.**: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) **Docket:** 6245.N DV1

Express Mall No.: EV 073687660 US

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Fig. 10A-147

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson Serial No.: Unassigned (Parent: 09/632,553) Filed: Herewith (Parent: Aug. 4, 2000) Docket: 6245.N DV1

Express Mall No.: EV 073687660 US

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116372974725111112711154167297501221773954704504859452495255888437280913748 0331100132140011021440060100001000100010001000101110101010

Fig. 10A-148

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

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Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

D cket: 6245.N DV1

Express Mail No.: EV 073687660 US

Filed: Herewith (Parent: Aug. 4, 2000) D cket: 6245.N DV1

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๚๎๚๎๚๎๚๎๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚๚
26753336850611118982931946329164416237875642270572432941468841035927493651 95684564556818645644945637096816763359756678567305865995457085937493651 1 2 1 11 1
5948565558847888695252184890819251591691594766941115288995886906768
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5752017670574628894485081732481737248587273647441540378825454109121010062 741004991148674122122669525072864715577077819640758927798724795884987246 11121 1713 7121122 1212111 111 2 11121 211161 17 7111
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3 12 23 232321 1 3 2 11111112113 1112 1331122 211332 13 11 22221 222
104559342078222103633240000005740502232831607562553691652671754067175029
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03363760489297141634444411237671157853866629369332175677828944456542315 2000000000000000000000000000000000000

Fig. 10A-150

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF STAPHYLOCOCCUS AUREUS THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial N .: Unassigned (Parent: 09/632,553)

Filed: Herewith (Parent: Aug. 4, 2000)

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Fig. 10A-151

Title: CRYSTALLIZATION AND STRUCTURE DETERMINATION OF *STAPHYLOCOCCUS AUREUS* THYMIDYLATE KINASE Applicant(s): Timothy E. Benson
Serial No.: Unassigned (Parent: 09/632,553)

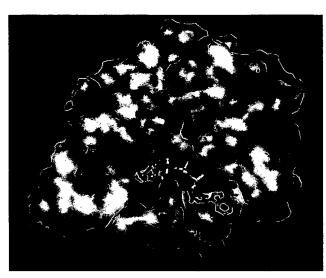
Filed: Herewith (Parent: Aug. 4, 2000)

Docket: 6245.N DV1

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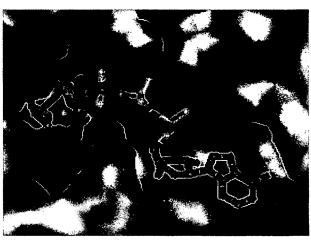


Fig. 11a





Fig. 11b

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